

The Influence of Temperature on Ozone Production under varying NO_x Conditions – a modelling study: Supplementary Material

J. Coates¹, K. Mar¹, N. Ojha² and T. Butler¹

¹Institute for Advanced Sustainability Studies, Potsdam, Germany

²Atmospheric Chemistry Department, Max Planck Institute for Chemistry, Mainz,
Germany

March 24, 2016

S1 Vertical Mixing with Diurnal Boundary Layer Height

The MECCA box model used in Coates and Butler (2015) included a constant boundary layer height of 1 km and no interactions (vertical mixing) with the free troposphere. In reality, the planetary boundary layer (PBL) height varies diurnally and affects chemistry by diluting emissions after sunrise when the PBL rises.

The evolution of the PBL leads to vertical mixing of the near surface air with the free tropospheric air mass. When the PBL collapses in the evening, pollutants are trapped in the PBL. The mixing layer height was measured as part of the BAERLIN campaign (Bonn et al., 2016) over Berlin, Germany. The profile of mean mixing layer height during the campaign period (June – August 2014) was used in the box model to represent the diurnal cycle of the mixing layer height. We implemented the vertical mixing scheme into the boxmodel following the approach of Lourens et al. (2016).

The mixing ratios of O₃, CO and CH₄ in the free troposphere were respectively set to 50 ppbv, 116 ppbv and 1.8 ppmv. These conditions were taken from the MATCH-MPIC chemical weather forecast model on the 21st March (the start date of the simulations). The model results (<http://cwf.iass-potsdam.de/>) at the 700 hPa height were chosen and the daily average was

25 used as input into the boxmodel.

26 **S2 Allocation of Benelux AVOC emissions to Mechanism** 27 **Species**

28 Anthropogenic NMVOC emissions over Benelux specified by the TNO_MACCIII emission
29 inventory (Kuenen et al., 2014) were translated to MCM v3.2 emissions (Table S1). The
30 MCM v3.2 emissions for each initial species were translated to emissions of mechanism species
31 into CRI v2, MOZART-4 and RADM2 chemical mechanisms by weighting with the carbon
32 numbers (Tables S2 – S4). The allocation of MCM v3.2 emissions into CB05 species followed the
33 recommendations of Yarwood et al. (2005) (Table S5).

Table S1: Speciated TNO_MACCIII emissions for Benelux AVOC and BVOC emissions (molecules cm⁻² s⁻¹) mapped to MCM v3.2 species (Kuenen et al., 2014).

Type	MCM.Species	SNAP.1	SNAP.2	SNAP.34	SNAP.5	SNAP.6	SNAP.71	SNAP.72	SNAP.73	SNAP.74	SNAP.8	SNAP.9	BVOC	Total
Ethane	C2H6	9.85e+08	1668300000	9.18e+09			9.67e+08	2.96e+08	638600000		3.45e+08	210200000		1.3728e+10
	C3H8	2.886e+09	1086600000	2.573e+09	1.041e+11	9.72e+08	470900000	2024000000	6386000000	627100000	2497000000	75200000		1.129e+11
Butanes	NC4H10	2.127e+09	882870000	9492700000	6.11e+11	3.61e+09	1.048e+09	2095000000		10378000000	3153000000	42200000		6.21e+11
	IC4H10	2586000000	3096600000	2323110000	1.486e+11	1637000000	4891000000	975000000		4839000000	1579000000	42200000		1.509e+11
Pentanes	NC5H12	1.783e+09	1014960000		4.548e+11		6.27e+08	8.4e+07		5215000000	1182000000	148900000		4.589e+11
	IC5H12	7.52e+08	544340000		2.718e+11		1.216e+09	1635000000		10117000000	2256000000	148900000		2.762e+11
	NEOP											148900000		148900000
	NC6H14	9541000000	573900000	1.211e+09	6.49e+10	3.162e+09	2.207e+09	1.246e+09		1934500000	4.26e+08	51600000		7.44e+10
Hexane and Higher Alkanes	M2PE			1566000000	9.98e+09	6.66e+08					7.08e+08	22150000		1.151e+10
	M3PE			1171000000	4.989e+09	6.66e+08					4.26e+08			6.2e+09
	NC7H16	4095200000	98740000	5.71e+08	6.97e+10	1.146e+09	3635000000	2053000000		317900000	1219000000	26040000		7.28e+10
	M2HEX					4.3e+08	2.83e+08	1595000000		247100000	1829000000			1.08e+09
	M3HEX					4.3e+08	2.02e+08	1.14e+08		17634000	1219000000			8.86e+08
	M22C4										1418000000			1418000000
	M23C4										1418000000			1418000000
	NC8H18			2353000000	5.18e+10	1256000000	3195000000	1797000000		278900000	6.95e+08	89000000		5.33e+10
	NC9H20			1312000000		3.02e+09						29690000		3.148e+09
	NC10H22			1.66e+08		5.85e+09	1422000000	803000000		124580000		44600000		6.25e+09
	NC11H24			646000000		2.387e+09	5183000000	2928000000		45360000	781000000	16250000		2.617e+09
	NC12H26					1685000000	8.45e+08	4769000000		741000000	717000000			1.637e+09
	CHEX		914900000	4e+07		6.82e+08						15060000		8.15e+08
Ethene	C2H4	2123000000	3695700000	3.368e+10			5.341e+09	3.807e+09	3425000000		4.62e+09	1.9e+08		5.188e+10
Propene	C3H6	1417000000	8682000000	6.59e+08			1.876e+09	6348000000	1518100000		7.86e+08	545000000		5.18e+09
Higher Alkenes	HEX1ENE	21050000	15773000									21810000		587030000
	BUT1ENE		22154000	2404000000							24510000			2866040000
	MEPROPENE													122600000
	TBUT2ENE										12260000			122600000
	CBUT2ENE										12260000			122600000
	CPENT2ENE		6961000								4902000			118610000
	TPENT2ENE		6961000								4902000			118610000
	PENT1ENE		6328000	6186000							19630000			321710000
	ME2BUT2ENE		3793000								9800000			135810000
	ME3BUT1ENE		3793000								9800000			135810000
	ME2BUT1ENE		2525500											2525500
Ethyne	C2H2	2697000	1252200000	4266000000			4.975e+09	1.795e+09	1346900000	2525000000	1.614e+09	71500000		1.051e+10
Benzene	BENZENE	2696000000	1.006e+09	8.3e+08	1.621e+10		1.197e+09	2283000000		35380000	2.83e+08	36540000		2.014e+10

Table S1: Speciated TNO_MACCIII emissions for Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped to MCM v3.2 species (Kuenen et al., 2014).

Type	MCM.Species	SNAP.1	SNAP.2	SNAP.34	SNAP.5	SNAP.6	SNAP.71	SNAP.72	SNAP.73	SNAP.74	SNAP.8	SNAP.9	BVOC	Total
Toluene	TOLUENE	252700000	372760000	84400000	1.375e+10	6.8e+09	2.708e+09	1.45e+08		30030000	193900000	24100000		2.435e+10
	MXYL	1.05e+08	21179000	1669300	1.994e+09	3.93e+09	5.77e+08	61040000		4735000	702000000	4880000		6.78e+09
	OXYL	233300000	21179000	669700	1.994e+09	9.84e+08	5.77e+08	61040000		4735000	571000000	2924000		3.717e+09
	PXYL		21179000	669700	1.994e+09	9.84e+08	432900000	45800000		3551000	702000000	3909000		3.556e+09
Trimethylbenzenes	TM123B	18550	1304500			6.6e+07	992000000				3330000	441000		170200000
	TM124B	18550	1304500	56100000		2246000000	4.16e+08				7760000	589000		7.06e+08
	TM135B	18550	1304500			6.6e+07	158600000				3330000	589000		2299000000
Other Aromatics	EBENZ	35100000		63400000		179400000	430600000	341600000	119530		8e+08	5250000		1.856e+09
	PBENZ					39600000	380600000	301500000	105570		128500000	2311000		8.53e+08
	IPBENZ					1453000000					128500000	2311000		2763000000
	PETHTOL					13210000					257500000			2703000000
	METHTOL					396000000					257500000			2963000000
	OETHTOL										192800000			1928000000
	DIET35TOL						8.05e+08	637600000	223800					1.443e+09
	DIME35EB					2247000000	993000000	78700000	27540					4.03e+08
	STYRENE			64600000		45700000	91500000	72500000	25440					2751000000
	BENZAL						153900000	121900000	42690					2759000000
Formaldehyde	PHENOL			71500000										715000000
	HCHO	611400000	2195300000				1.177e+09	1.781e+09	85260000		2.9e+09	29490000		8.77e+09
	CH3CHO	11780000	130090000	73750000			318400000	7.39e+08	16383000		6.8e+08	6860000		1.976e+09
	C2H5CHO	6710000	98630000				53670000	124600000	2752000		257700000	5200000		5.49e+08
	C3H7CHO	38630	79420000								207600000	4190000		2921000000
	IPRCHO	38630	79420000								138400000	4190000		2221000000
	C4H9CHO	32340	66550000									3504000		700500000
	ACR	49770	102260000				83300000	193800000	4282000			5390000		3888000000
	MACR	39730	81710000									4310000		861100000
	C4ALDB	39730	81710000				44510000	103300000	2287000			4310000		2361000000
Alkadienes and Other Alkynes	MGLYOX									138500000				1385000000
	C4H6	67600000	771300000	4.74e+09	2.221e+11		2.505e+09	7.78e+08	245800000	458800000	1.033e+09	52800000	1.435e+10	2.332e+11
	C5H8													
	HCOOH	4660000	1201400000								1.67e+08	69400000		14424000000
Organic Acids	CH3CO2H	3572000	9.21e+08	167700000							1.28e+08	53200000		1.274e+09
	PROPACID	2898000	746100000								1.04e+08	43100000		8971000000
	ACO2H			140400000										1404000000

Table S1: Speciated TNO_MACCIII emissions for Benelux AVOC and BVOC emissions (molecules cm⁻² s⁻¹) mapped to MCM v3.2 species (Kuenen et al., 2014).

Type	MCM.Species	SNAP.1	SNAP.2	SNAP.34	SNAP.5	SNAP.6	SNAP.71	SNAP.72	SNAP.73	SNAP.74	SNAP.8	SNAP.9	BVOC	Total
Alcohols	CH3OH	140000		3200000		6.38e+09				40419000	24020000			6.45e+09
	C2H5OH	97400	1.687e+09	903000000		6.52e+09				28082900	633000000			8.39e+09
	NPROPOL	74600				5.31e+08				21563500	7670000			5.61e+08
	IPROPOL	74600		1135000		8.49e+08				21563500				8.73e+08
	NBUTOL	60500				5.17e+08				17451500				5.34e+08
	BUT2OL	60500				345400000				17451500	10360000			3.73e+08
	IBUTOL	60500				215300000				17451500				232800000
	TBUTOL	60500								17451500				17489700
	PECOH	50900								14643300				14775400
	IPEAOH	50900								14643300				14775400
	ME3BUOL	50900								14643300				14775400
	IPECOH	50900								14643300				14775400
	IPEBOH	50900								14643300				14775400
	CYHEXOL	44800								12938100				12966400
	MIBKAOH	38600				1099000000				11132900				121100000
	ETHGLY	72300				154300000				20861500				175200000
	PROPGLY	59000				307800000				16950200				324800000
	C6H5CH2OH					88500000								88500000
	MBO	52100								15044300				15077200
Ketones	CH3COCH3	384100	15896000	6.38e+08		6.66e+09	35750000	229900000		382100000	1414000			7.96e+09
	MEK		12828000			3.212e+09					1139000			3.236e+09
	MPRK		10745000								954000			11705000
	DIEK		10745000								954000			11705000
	MPK		10745000								954000			11705000
	HEX2ONE		9242000								820000			10062000
	HEX3ONE		9242000								820000			10062000
	MIBK		9242000			1.93e+09					820000			1.94e+09
	MTBK		9242000								820000			10062000
	CYHEXONE		9439000	34310000		157500000					837000			202200000
	APINENE											3050000	1.835e+09	1.839e+09
	BPINENE											3050000	1.835e+09	1.839e+09
	LIMONENE					209500000					4580000		1.835e+09	2.046e+09
Esters	METHACET			64470000										64470000
	ETHACET			7386000		4.44e+09								4.45e+09
	NBUTACET					3.113e+09								3.113e+09
	IPOACET					1.095e+09								1.095e+09

Table S1: Speciated TNO_MACCIII emissions for Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped to MCM v3.2 species (Kuenen et al., 2014).

Type	MCM.Species	SNAP.1	SNAP.2	SNAP.34	SNAP.5	SNAP.6	SNAP.71	SNAP.72	SNAP.73	SNAP.74	SNAP.8	SNAP.9	BVOC	Total
Ethers	CH3OCHO			7229000								7950000		7229000
	NPROACET					4.1e+08								4.18e+08
	CH3OCH3	61750000	253500000			244300000								5.59e+08
	DIETETHER	38360000	94510000											132360000
	MTBE	32330000												32330000
	DIIPREETHER	27860000	68540000									19520000		115960000
	ETBE	27860000												27860000
	MO2EOL	37420000				295700000								3.33e+08
	EOX2EOL	31600000				249900000								281500000
	PR2OHMOX	31600000				5e+08								5.32e+08
	BUOX2ETOH	24117000				2.398e+09								2.422e+09
	BOX2PROL	21510000												21510000
	CH2CL2		6.74e+08			1.589e+09						1458000		2.262e+09
	CH3CH2CL		5.22e+08											5.22e+08
Chlorinated Hydrocarbons	CH3CCL3					1.113e+09						464000		1.114e+09
	TRICLETH		256600000			2.516e+09						471000		2.776e+09
	CDICLETH		173100000									951000		174800000
	TDICLETH		173100000									634000		174600000
	CH3CL		5.34e+08											5.34e+08
	CCL2CH2		173100000											173100000
	CHCL2CH3											715000		715000
	VINCL		1.62e+08											1.62e+08
	TCE		40500000			6.11e+08						927000		6.53e+08
	CHCL3		112800000											112800000
Total		1.192e+10	2.1806e+10	6.11e+10	2.049e+12	8.39e+10	3.33e+10	1.581e+10	1688300000	4.285e+09	2.059e+10	1.333e+09	1.9847e+10	2.32e+12

Table S2: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to CRIv2 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	CRIv2 Species	Belgium	Netherlands	Luxembourg	Total
Ethane	C2H6	C2H6	4.91E+09	8.58E+08	7.96E+09	1.37E+10
Propane	C3H8	C3H8	3.35E+10	4.00E+10	3.94E+10	1.13E+11
Butanes	NC4H10	NC4H10	1.25E+11	3.49E+11	1.47E+11	6.21E+11
	IC4H10	IC4H10	3.03E+10	8.50E+10	3.56E+10	1.51E+11
Pentanes	NC5H12	NC5H12	8.89E+10	2.65E+11	1.05E+11	4.59E+11
	IC5H12	IC5H12	5.33E+10	1.60E+11	6.29E+10	2.76E+11
	NEOP	NEOP	1.11E+07	0.00E+00	3.79E+06	1.49E+07
Hexane and Higher Alkanes	NC6H14	NC6H14	1.52E+10	4.10E+10	1.82E+10	7.44E+10
	M2PE	M2PE	2.39E+09	6.28E+09	2.84E+09	1.15E+10
	M3PE	M3PE	1.34E+09	3.29E+09	1.57E+09	6.20E+09
	NC7H16	NC7H16	1.45E+10	4.12E+10	1.71E+10	7.28E+10
	M2HEX	M2HEX	2.74E+08	4.89E+08	3.17E+08	1.08E+09
	M3HEX	M3HEX	2.37E+08	3.90E+08	2.59E+08	8.86E+08
	M22C4	M22C4	3.47E+07	5.29E+07	5.42E+07	1.42E+08
	M23C4	M23C4	3.47E+07	5.29E+07	5.42E+07	1.42E+08
	NC8H18	NC8H18	1.04E+10	3.06E+10	1.23E+10	5.33E+10
	NC9H20	NC9H20	1.10E+09	1.07E+09	9.78E+08	3.15E+09
	NC10H22	NC10H22	2.15E+09	2.21E+09	1.89E+09	6.25E+09
	NC11H24	NC11H24	8.95E+08	9.26E+08	7.96E+08	2.62E+09
	NC12H26	NC12H26	3.07E+08	8.88E+08	4.42E+08	1.64E+09
	CHEX	CHEX	2.91E+08	2.44E+08	2.80E+08	8.15E+08
Ethene	C2H4	C2H4	3.66E+10	7.03E+09	8.25E+09	5.19E+10
Propene	C3H6	C3H6	1.82E+09	1.68E+09	1.68E+09	5.18E+09
Higher Alkenes	HEX1ENE	HEX1ENE	3.42E+07	5.03E+05	2.40E+07	5.87E+07
	BUT1ENE	BUT1ENE	9.99E+07	7.04E+05	1.86E+08	2.87E+08
	MEPROPENE	MEPROPENE	9.80E+06	0.00E+00	2.46E+06	1.23E+07
	TBUT2ENE	TBUT2ENE	9.80E+06	0.00E+00	2.46E+06	1.23E+07
	CBUT2ENE	CBUT2ENE	9.80E+06	0.00E+00	2.46E+06	1.23E+07
	CPENT2ENE	CPENT2ENE	9.57E+06	2.21E+05	2.07E+06	1.19E+07
	TPENT2ENE	TPENT2ENE	9.57E+06	2.21E+05	2.07E+06	1.19E+07
	PENT1ENE	PENT1ENE	2.68E+07	2.01E+05	5.17E+06	3.22E+07
	ME2BUT2ENE	ME2BUT2ENE	1.09E+07	1.21E+05	2.56E+06	1.36E+07
	ME3BUT1ENE	ME3BUT1ENE	1.09E+07	1.21E+05	2.56E+06	1.36E+07
	ME2BUT1ENE	ME2BUT1ENE	2.05E+06	8.05E+04	3.95E+05	2.53E+06
Ethyne	C2H2	C2H2	2.78E+09	4.51E+09	3.22E+09	1.05E+10

Table S2: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to CRIv2 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	CRIv2 Species	Belgium	Netherlands	Luxembourg	Total
Benzene	BENZENE	BENZENE	4.52E+09	1.06E+10	5.02E+09	2.01E+10
Toluene	TOLUENE	TOLUENE	5.78E+09	1.22E+10	6.37E+09	2.44E+10
Xylenes	MXYL	MXYL	1.90E+09	3.00E+09	1.88E+09	6.78E+09
	OXYL	OXYL	8.61E+08	1.89E+09	9.66E+08	3.72E+09
	PXYL	PXYL	8.28E+08	1.82E+09	9.08E+08	3.56E+09
Trimethylbenzenes	TM123B	TM123B	4.49E+07	7.36E+07	5.17E+07	1.70E+08
	TM124B	TM124B	1.75E+08	2.89E+08	2.42E+08	7.06E+08
	TM135B	TM135B	5.58E+07	1.03E+08	7.11E+07	2.30E+08
Other Aromatics	EBENZ	EBENZ	3.99E+08	8.28E+08	6.29E+08	1.86E+09
	PBENZ	PBENZ	1.59E+08	4.63E+08	2.31E+08	8.53E+08
	IPBENZ	IPBENZ	7.88E+07	1.04E+08	9.35E+07	2.76E+08
	PETHTOL	PETHTOL	6.03E+07	1.05E+08	1.05E+08	2.70E+08
	METHTOL	METHTOL	6.93E+07	1.14E+08	1.13E+08	2.96E+08
	OETHTOL	OETHTOL	4.19E+07	7.47E+07	7.62E+07	1.93E+08
	DIET35TOL	DIET35TOL	2.45E+08	8.42E+08	3.56E+08	1.44E+09
	DIME35EB	DIME35EB	1.06E+08	1.88E+08	1.09E+08	4.03E+08
	STYRENE	STYRENE	6.01E+07	1.13E+08	1.02E+08	2.75E+08
	BENZAL	BENZAL	4.68E+07	1.61E+08	6.81E+07	2.76E+08
	PHENOL	AROH14	1.86E+07	0.00E+00	5.29E+07	7.15E+07
Formaldehyde	HCHO	HCHO	2.35E+09	3.04E+09	3.38E+09	8.77E+09
Other Aldehydes	CH3CHO	CH3CHO	5.53E+08	8.88E+08	5.35E+08	1.98E+09
	C2H5CHO	C2H5CHO	1.78E+08	1.97E+08	1.74E+08	5.49E+08
	C3H7CHO	C3H7CHO	1.19E+08	6.71E+07	1.06E+08	2.92E+08
	IPRCHO	IPRCHO	9.60E+07	4.57E+07	8.04E+07	2.22E+08
	C4H9CHO	C4H9CHO	4.25E+07	2.45E+06	2.51E+07	7.01E+07
	ACR	UCARB10	8.33E+07	1.35E+08	7.33E+07	2.92E+08
	MACR	UCARB10	5.23E+07	3.01E+06	3.08E+07	8.61E+07
	C4ALDB	UCARB10	7.67E+07	9.70E+07	6.24E+07	2.36E+08
	MGLYOX	CARB6	4.52E+07	2.85E+07	3.36E+07	1.07E+08
Alkadienes and	C4H6	C4H6	4.36E+10	1.34E+11	5.56E+10	2.33E+11
Other Alkynes	C5H8	C5H8	3.35E+09	1.10E+10	0.00E+00	1.44E+10
Organic Acids	HCOOH	HCOOH	9.28E+08	4.04E+07	4.74E+08	1.44E+09
	CH3CO2H	CH3CO2H	7.55E+08	3.10E+07	4.88E+08	1.27E+09
	PROPACID	PROPACID	5.77E+08	2.51E+07	2.95E+08	8.97E+08
	ACO2H	PROPACID	3.64E+07	0.00E+00	1.04E+08	1.40E+08

Table S2: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to CRIv2 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	CRIv2 Species	Belgium	Netherlands	Luxembourg	Total
Alcohols	CH3OH	CH3OH	2.20E+09	2.40E+09	1.85E+09	6.45E+09
	C2H5OH	C2H5OH	3.30E+09	2.51E+09	2.58E+09	8.39E+09
	NPROPOL	NPROPOL	2.06E+08	2.00E+08	1.55E+08	5.61E+08
	IPROPOL	IPROPOL	3.08E+08	3.19E+08	2.46E+08	8.73E+08
	NBUTOL	NBUTOL	1.91E+08	1.94E+08	1.49E+08	5.34E+08
	BUT2OL	BUT2OL	1.41E+08	1.30E+08	1.02E+08	3.73E+08
	IBUTOL	IBUTOL	8.97E+07	8.09E+07	6.22E+07	2.33E+08
	TBUTOL	TBUTOL	1.74E+07	0.00E+00	8.97E+04	1.75E+07
	PECOH	PECOH	1.47E+07	0.00E+00	7.54E+04	1.48E+07
	IPEAOH	IPEAOH	1.47E+07	0.00E+00	7.54E+04	1.48E+07
	ME3BUOL	ME3BUOL	1.47E+07	0.00E+00	7.54E+04	1.48E+07
	IPECOH	IPECOH	1.47E+07	0.00E+00	7.54E+04	1.48E+07
	IPEBOH	IPEBOH	1.47E+07	0.00E+00	7.54E+04	1.48E+07
	CYHEXOL	CYHEXOL	1.29E+07	0.00E+00	6.64E+04	1.30E+07
	MIBKAOH	MIBKAOH	4.80E+07	4.13E+07	3.18E+07	1.21E+08
	ETHGLY	ETHGLY	7.26E+07	5.80E+07	4.46E+07	1.75E+08
	PROPGLY	PROPGLY	1.20E+08	1.16E+08	8.88E+07	3.25E+08
	C6H5CH2OH	BENZAL	2.31E+07	2.59E+07	1.99E+07	6.89E+07
	MBO	PENT1ENE	1.50E+07	0.00E+00	7.72E+04	1.51E+07
Ketones	CH3COCH3	CH3COCH3	2.67E+09	2.75E+09	2.54E+09	7.96E+09
	MEK	MEK	1.11E+09	1.20E+09	9.26E+08	3.24E+09
	MPRK	MPRK	8.03E+06	3.75E+05	3.30E+06	1.17E+07
	DIEK	DIEK	8.03E+06	3.75E+05	3.30E+06	1.17E+07
	MIPK	MIPK	8.03E+06	3.75E+05	3.30E+06	1.17E+07
	HEX2ONE	HEX2ONE	6.90E+06	3.22E+05	2.84E+06	1.01E+07
	HEX3ONE	HEX3ONE	6.90E+06	3.22E+05	2.84E+06	1.01E+07
	MIBK	MIBK	6.67E+08	7.17E+08	5.56E+08	1.94E+09
	MTBK	MTBK	6.90E+06	3.22E+05	2.84E+06	1.01E+07
	CYHEXONE	CYHEXONE	6.99E+07	5.89E+07	7.34E+07	2.02E+08
Esters	METHACET	METHACET	6.18E+07	0.00E+00	2.67E+06	6.45E+07
	ETHACET	ETHACET	1.48E+09	1.68E+09	1.29E+09	4.45E+09
	NBUTACET	NBUTACET	1.03E+09	1.18E+09	9.03E+08	3.11E+09
	IPROACET	IPROACET	3.63E+08	4.14E+08	3.18E+08	1.10E+09
	CH3OCHO	CH3OCHO	6.93E+06	0.00E+00	2.99E+05	7.23E+06
	NPROACET	NPROACET	1.42E+08	1.55E+08	1.21E+08	4.18E+08

Table S2: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to CRIv2 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	CRIv2 Species	Belgium	Netherlands	Luxembourg	Total
Ethers	CH3OCH3	CH3OCH3	3.59E+08	9.30E+07	1.07E+08	5.59E+08
	DIETETHER	DIETETHER	1.11E+08	1.46E+06	1.99E+07	1.32E+08
	MTBE	MTBE	1.76E+07	1.23E+06	1.35E+07	3.23E+07
	DIIPREETHER	DIIPREETHER	9.56E+07	1.06E+06	1.93E+07	1.16E+08
	ETBE	ETBE	1.52E+07	1.06E+06	1.16E+07	2.79E+07
	MO2EOL	MO2EOL	1.21E+08	1.11E+08	1.01E+08	3.33E+08
	EOX2EOL	EOX2EOL	1.02E+08	9.39E+07	8.56E+07	2.82E+08
	PR2OHMOX	PR2OHMOX	1.87E+08	1.87E+08	1.58E+08	5.32E+08
	BUOX2ETOH	BUOX2ETOH	8.27E+08	8.90E+08	7.05E+08	2.42E+09
	BOX2PROL	BOX2PROL	1.17E+07	8.20E+05	8.99E+06	2.15E+07
Chlorinated Hydrocarbons	CH2CL2	C2H2	4.17E+08	2.04E+08	5.12E+08	1.13E+09
	CH3CH2CL	C2H2	1.36E+08	0.00E+00	3.86E+08	5.22E+08
	CH3CCL3	C2H2	4.61E+08	2.86E+08	3.67E+08	1.11E+09
	TRICLETH	C2H4	1.11E+09	6.46E+08	1.02E+09	2.78E+09
	CDICLETH	C2H4	4.58E+07	0.00E+00	1.29E+08	1.75E+08
	TDICLETH	C2H4	4.56E+07	0.00E+00	1.29E+08	1.75E+08
	CH3CL	C2H2	6.93E+07	0.00E+00	1.97E+08	2.66E+08
	CCL2CH2	C2H4	4.51E+07	0.00E+00	1.28E+08	1.73E+08
	CHCL2CH3	C2H2	5.35E+05	0.00E+00	1.80E+05	7.15E+05
	VINCL	C2H4	4.20E+07	0.00E+00	1.20E+08	1.62E+08
	TCE	C2H4	2.64E+08	1.57E+08	2.32E+08	6.53E+08
	CHCL3	C2H4	1.47E+07	0.00E+00	4.17E+07	5.64E+07
Terpenes	APINENE	APINENE	4.22E+08	1.27E+09	1.47E+08	1.84E+09
	BPINENE	BPINENE	4.22E+08	1.27E+09	1.47E+08	1.84E+09
	LIMONENE	APINENE	4.96E+08	1.34E+09	2.10E+08	2.05E+09
Total			5.15E+11	1.25E+12	5.64E+11	2.32E+12

Table S3: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to MOZART-4 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	MOZART-4 Species	Belgium	Netherlands	Luxembourg	Total
Ethane	C2H6	C2H6	4.91E+09	8.58E+08	7.96E+09	1.37E+10
Propane	C3H8	C3H8	3.35E+10	4.00E+10	3.94E+10	1.13E+11
Butanes	NC4H10	BIGALK	1.00E+11	2.79E+11	1.17E+11	4.96E+11
	IC4H10	BIGALK	2.42E+10	6.80E+10	2.85E+10	1.21E+11
Pentanes	NC5H12	BIGALK	8.89E+10	2.65E+11	1.05E+11	4.59E+11
	IC5H12	BIGALK	5.33E+10	1.60E+11	6.29E+10	2.76E+11
	NEOP	BIGALK	1.11E+07	0.00E+00	3.79E+06	1.49E+07
Hexane and Higher Alkanes	NC6H14	BIGALK	1.82E+10	4.92E+10	2.18E+10	8.92E+10
	M2PE	BIGALK	2.87E+09	7.54E+09	3.41E+09	1.38E+10
	M3PE	BIGALK	1.61E+09	3.94E+09	1.89E+09	7.44E+09
	NC7H16	BIGALK	2.02E+10	5.77E+10	2.39E+10	1.02E+11
	M2HEX	BIGALK	3.83E+08	6.84E+08	4.44E+08	1.51E+09
	M3HEX	BIGALK	3.31E+08	5.45E+08	3.63E+08	1.24E+09
	M22C4	BIGALK	4.16E+07	6.34E+07	6.51E+07	1.70E+08
	M23C4	BIGALK	4.16E+07	6.34E+07	6.51E+07	1.70E+08
	NC8H18	BIGALK	1.67E+10	4.89E+10	1.97E+10	8.53E+10
	NC9H20	BIGALK	1.99E+09	1.93E+09	1.76E+09	5.68E+09
	NC10H22	BIGALK	4.31E+09	4.42E+09	3.78E+09	1.25E+10
	NC11H24	BIGALK	1.97E+09	2.04E+09	1.75E+09	5.76E+09
	NC12H26	BIGALK	7.37E+08	2.13E+09	1.06E+09	3.93E+09
	CHEX	BIGALK	3.49E+08	2.93E+08	3.36E+08	9.78E+08
Ethene	C2H4	C2H4	3.66E+10	7.03E+09	8.25E+09	5.19E+10
Propene	C3H6	C3H6	1.82E+09	1.68E+09	1.68E+09	5.18E+09
Higher Alkenes	HEX1ENE	BIGENE	5.13E+07	7.55E+05	3.60E+07	8.81E+07
	BUT1ENE	BIGENE	9.99E+07	7.04E+05	1.86E+08	2.87E+08
	MEPROPENE	BIGENE	9.80E+06	0.00E+00	2.46E+06	1.23E+07
	TBUT2ENE	BIGENE	9.80E+06	0.00E+00	2.46E+06	1.23E+07
	CBUT2ENE	BIGENE	9.80E+06	0.00E+00	2.46E+06	1.23E+07
	CPENT2ENE	BIGENE	1.20E+07	2.77E+05	2.58E+06	1.49E+07
	TPENT2ENE	BIGENE	1.20E+07	2.77E+05	2.58E+06	1.49E+07
	PENT1ENE	BIGENE	3.34E+07	2.52E+05	6.47E+06	4.01E+07
	ME2BUT2ENE	BIGENE	1.37E+07	1.51E+05	3.20E+06	1.71E+07
	ME3BUT1ENE	BIGENE	1.37E+07	1.51E+05	3.20E+06	1.71E+07
	ME2BUT1ENE	BIGENE	2.57E+06	1.01E+05	4.93E+05	3.16E+06
Ethyne	C2H2	C2H2	2.78E+09	4.51E+09	3.22E+09	1.05E+10

Table S3: Benelux AVOC and BVOC emissions (molecules cm⁻² s⁻¹) mapped from MCMv3.2 species to MOZART-4 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	MOZART-4 Species	Belgium	Netherlands	Luxembourg	Total
Benzene	BENZENE	TOLUENE	3.87E+09	9.05E+09	4.30E+09	1.72E+10
Toluene	TOLUENE	TOLUENE	5.78E+09	1.22E+10	6.37E+09	2.44E+10
Xylenes	MXYL	TOLUENE	2.17E+09	3.43E+09	2.14E+09	7.74E+09
	OXYL	TOLUENE	9.85E+08	2.16E+09	1.10E+09	4.25E+09
	PXYL	TOLUENE	9.46E+08	2.08E+09	1.04E+09	4.07E+09
Trimethylbenzenes	TM123B	TOLUENE	5.78E+07	9.47E+07	6.65E+07	2.19E+08
	TM124B	TOLUENE	2.25E+08	3.72E+08	3.12E+08	9.09E+08
	TM135B	TOLUENE	7.17E+07	1.32E+08	9.14E+07	2.95E+08
Other Aromatics	EBENZ	TOLUENE	4.57E+08	9.46E+08	7.19E+08	2.12E+09
	PBENZ	TOLUENE	2.04E+08	5.95E+08	2.97E+08	1.10E+09
	IPBENZ	TOLUENE	1.01E+08	1.34E+08	1.20E+08	3.55E+08
	PETHTOL	TOLUENE	7.76E+07	1.34E+08	1.36E+08	3.48E+08
	METHTOL	TOLUENE	8.90E+07	1.47E+08	1.45E+08	3.81E+08
	OETHTOL	TOLUENE	5.39E+07	9.61E+07	9.80E+07	2.48E+08
	DIET35TOL	TOLUENE	3.84E+08	1.32E+09	5.60E+08	2.26E+09
	DIME35EB	TOLUENE	1.52E+08	2.68E+08	1.56E+08	5.76E+08
	STYRENE	TOLUENE	7.72E+07	1.45E+08	1.31E+08	3.53E+08
	BENZAL	TOLUENE	6.01E+07	2.07E+08	8.76E+07	3.55E+08
	PHENOL	TOLUENE	1.59E+07	0.00E+00	4.54E+07	6.13E+07
Formaldehyde	HCHO	CH2O	2.35E+09	3.04E+09	3.38E+09	8.77E+09
Other Aldehydes	CH3CHO	CH3CHO	5.53E+08	8.88E+08	5.35E+08	1.98E+09
	C2H5CHO	CH3CHO	2.67E+08	2.95E+08	2.61E+08	8.23E+08
	C3H7CHO	CH3CHO	2.37E+08	1.34E+08	2.11E+08	5.82E+08
	IPRCHO	CH3CHO	1.92E+08	9.14E+07	1.61E+08	4.44E+08
	C4H9CHO	CH3CHO	1.06E+08	6.13E+06	6.27E+07	1.75E+08
	ACR	MACR	8.33E+07	1.35E+08	7.33E+07	2.92E+08
	MACR	MACR	5.23E+07	3.01E+06	3.08E+07	8.61E+07
	C4ALDB	MACR	7.67E+07	9.70E+07	6.24E+07	2.36E+08
	MGLYOX	CH3COCHO	4.52E+07	4.28E+07	5.05E+07	1.39E+08
Alkadienes and	C4H6	BIGENE	4.36E+10	1.34E+11	4.45E+10	2.22E+11
Other Alkynes	C5H8	ISOP	3.35E+09	1.10E+10	0.00E+00	1.44E+10
Organic Acids	HCOOH	HCOOH	9.28E+08	4.04E+07	4.74E+08	1.44E+09
	CH3CO2H	CH3COOH	7.55E+08	3.10E+07	4.88E+08	1.27E+09
	PROPACID	CH3COOH	8.65E+08	3.77E+07	4.42E+08	1.34E+09
	ACO2H	CH3COOH	5.46E+07	0.00E+00	1.56E+08	2.11E+08

Table S3: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to MOZART-4 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	MOZART-4 Species	Belgium	Netherlands	Luxembourg	Total
Alcohols	CH3OH	CH3OH	2.20E+09	2.40E+09	1.85E+09	6.45E+09
	C2H5OH	C2H5OH	3.30E+09	2.51E+09	2.58E+09	8.39E+09
	NPROPOL	C2H5OH	3.08E+08	3.00E+08	2.33E+08	8.41E+08
	IPROPOL	C2H5OH	4.61E+08	4.79E+08	3.69E+08	1.31E+09
	NBUTOL	C2H5OH	3.82E+08	3.89E+08	2.98E+08	1.07E+09
	BUT2OL	C2H5OH	2.82E+08	2.59E+08	2.04E+08	7.45E+08
	IBUTOL	C2H5OH	1.79E+08	1.62E+08	1.24E+08	4.65E+08
	TBUTOL	C2H5OH	3.48E+07	0.00E+00	1.79E+05	3.50E+07
	PECOH	C2H5OH	3.66E+07	0.00E+00	1.88E+05	3.68E+07
	IPEAOH	C2H5OH	3.66E+07	0.00E+00	1.88E+05	3.68E+07
	ME3BUOL	C2H5OH	3.66E+07	0.00E+00	1.88E+05	3.68E+07
	IPECOH	C2H5OH	3.66E+07	0.00E+00	1.88E+05	3.68E+07
	IPEBOH	C2H5OH	3.66E+07	0.00E+00	1.88E+05	3.68E+07
	CYHEXOL	C2H5OH	3.87E+07	0.00E+00	1.99E+05	3.89E+07
	MIBKAOH	C2H5OH	1.44E+08	1.24E+08	9.53E+07	3.63E+08
	ETHGLY	C2H5OH	7.26E+07	5.80E+07	4.46E+07	1.75E+08
	PROPGLY	C2H5OH	1.80E+08	1.73E+08	1.33E+08	4.86E+08
	C6H5CH2OH	C2H5OH	1.04E+08	1.17E+08	8.94E+07	3.10E+08
	MBO	C2H5OH	3.75E+07	0.00E+00	1.93E+05	3.77E+07
Ketones	CH3COCH3	CH3COCH3	2.67E+09	2.75E+09	2.54E+09	7.96E+09
	MEK	MEK	1.11E+09	1.20E+09	9.26E+08	3.24E+09
	MPRK	MEK	1.00E+07	4.69E+05	4.12E+06	1.46E+07
	DIEK	MEK	1.00E+07	4.69E+05	4.12E+06	1.46E+07
	MIPK	MEK	1.00E+07	4.69E+05	4.12E+06	1.46E+07
	HEX2ONE	MEK	1.04E+07	4.84E+05	4.25E+06	1.51E+07
	HEX3ONE	MEK	1.04E+07	4.84E+05	4.25E+06	1.51E+07
	MIBK	MEK	1.00E+09	1.08E+09	8.34E+08	2.91E+09
	MTBK	MEK	1.04E+07	4.84E+05	4.25E+06	1.51E+07
	CYHEXONE	MEK	1.05E+08	8.83E+07	1.10E+08	3.03E+08
Esters	METHACET	BIGALK	3.71E+07	0.00E+00	4.08E+08	4.45E+08
	ETHACET	BIGALK	1.18E+09	1.35E+09	5.15E+07	2.58E+09
	NBUTACET	BIGALK	1.24E+09	1.41E+09	5.15E+07	2.70E+09
	IPROACET	BIGALK	3.63E+08	4.14E+08	7.90E+07	8.56E+08
	CH3OCHO	BIGALK	6.93E+06	0.00E+00	5.14E+07	5.83E+07
	NPROACET	BIGALK	1.42E+08	1.55E+08	7.22E+04	2.97E+08

Table S3: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to MOZART-4 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	MOZART-4 Species	Belgium	Netherlands	Luxembourg	Total
Ethers	CH3OCH3	BIGALK	1.44E+08	3.72E+07	1.47E+08	3.28E+08
	DIETETHER	BIGALK	8.92E+07	1.17E+06	1.47E+08	2.37E+08
	MTBE	BIGALK	1.76E+07	1.23E+06	2.10E+08	2.29E+08
	DIIPREETHER	BIGALK	1.15E+08	1.27E+06	1.60E+06	1.18E+08
	ETBE	BIGALK	1.82E+07	1.27E+06	1.03E+09	1.05E+09
	MO2EOL	BIGALK	7.25E+07	6.67E+07	1.08E+09	1.22E+09
	EOX2EOL	BIGALK	8.16E+07	7.51E+07	3.18E+08	4.75E+08
	PR2OHMOX	BIGALK	1.49E+08	1.49E+08	2.99E+05	2.98E+08
	BUOX2ETOH	BIGALK	9.92E+08	1.07E+09	1.21E+08	2.18E+09
	BOX2PROL	BIGALK	1.64E+07	1.15E+06	4.28E+07	6.04E+07
Chlorinated Hydrocarbons	CH2CL2	BIGALK	1.67E+08	8.16E+07	1.60E+07	2.65E+08
	CH3CH2CL	BIGALK	5.42E+07	0.00E+00	1.35E+07	6.77E+07
	CH3CCL3	BIGALK	1.84E+08	1.14E+08	2.32E+07	3.21E+08
	TRICLETH	BIGALK	4.43E+08	2.58E+08	1.40E+07	7.15E+08
	CDICLETH	BIGALK	1.83E+07	0.00E+00	6.08E+07	7.91E+07
	TDICLETH	BIGALK	1.82E+07	0.00E+00	6.85E+07	8.67E+07
	CH3CL	BIGALK	2.77E+07	0.00E+00	1.26E+08	1.54E+08
	CCL2CH2	BIGALK	1.80E+07	0.00E+00	8.46E+08	8.64E+08
	CHCL2CH3	BIGALK	2.14E+05	0.00E+00	1.26E+07	1.28E+07
	VINCL	BIGALK	1.68E+07	0.00E+00	2.05E+08	2.22E+08
	TCE	BIGALK	1.06E+08	6.27E+07	1.54E+08	3.23E+08
	CHCL3	BIGALK	5.86E+06	0.00E+00	1.47E+08	1.53E+08
Terpenes	APINENE	C10H16	4.22E+08	1.27E+09	4.78E+07	1.74E+09
	BPINENE	C10H16	4.22E+08	1.27E+09	9.26E+07	1.78E+09
	LIMONENE	C10H16	4.96E+08	1.34E+09	1.67E+07	1.85E+09
Total			5.05E+11	1.21E+12	5.39E+11	2.25E+12

Table S4: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to RADM2 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	RADM2 Species	Belgium	Netherlands	Luxembourg	Total
Ethane	C2H6	ETH	4.91E+09	8.58E+08	7.96E+09	1.37E+10
Propane	C3H8	HC3	3.47E+10	4.13E+10	4.08E+10	1.17E+11
Butanes	NC4H10	HC3	1.73E+11	4.81E+11	2.02E+11	8.56E+11
	IC4H10	HC3	4.18E+10	1.17E+11	4.91E+10	2.08E+11
Pentanes	NC5H12	HC5	9.26E+10	2.76E+11	1.09E+11	4.78E+11
	IC5H12	HC5	5.55E+10	1.66E+11	6.55E+10	2.87E+11
	NEOP	HC3	1.91E+07	0.00E+00	6.54E+06	2.56E+07
Hexane and Higher Alkanes	NC6H14	HC5	1.89E+10	5.12E+10	2.28E+10	9.29E+10
	M2PE	HC5	2.99E+09	7.85E+09	3.55E+09	1.44E+10
	M3PE	HC5	1.67E+09	4.11E+09	1.97E+09	7.75E+09
	NC7H16	HC5	2.11E+10	6.01E+10	2.49E+10	1.06E+11
	M2HEX	HC8	2.42E+08	4.33E+08	2.81E+08	9.56E+08
	M3HEX	HC8	2.10E+08	3.45E+08	2.30E+08	7.85E+08
	M22C4	HC3	7.18E+07	1.09E+08	1.12E+08	2.93E+08
	M23C4	HC5	4.34E+07	6.61E+07	6.78E+07	1.77E+08
	NC8H18	HC8	1.06E+10	3.10E+10	1.25E+10	5.41E+10
	NC9H20	HC8	1.26E+09	1.22E+09	1.11E+09	3.59E+09
	NC10H22	HC8	2.73E+09	2.80E+09	2.39E+09	7.92E+09
	NC11H24	HC8	1.25E+09	1.29E+09	1.11E+09	3.65E+09
	NC12H26	HC8	4.66E+08	1.35E+09	6.71E+08	2.49E+09
	CHEX	HC8	2.21E+08	1.85E+08	2.13E+08	6.19E+08
Ethene	C2H4	OL2	3.66E+10	7.03E+09	8.25E+09	5.19E+10
Propene	C3H6	OLT	1.43E+09	1.32E+09	1.32E+09	4.07E+09
Higher Alkenes	HEX1ENE	OLT	5.40E+07	7.94E+05	3.79E+07	9.27E+07
	BUT1ENE	OLT	1.05E+08	7.41E+05	1.96E+08	3.02E+08
	MEPROPENE	OLI	8.17E+06	0.00E+00	2.05E+06	1.02E+07
	TBUT2ENE	OLI	8.17E+06	0.00E+00	2.05E+06	1.02E+07
	CBUT2ENE	OLI	8.17E+06	0.00E+00	2.05E+06	1.02E+07
	CPENT2ENE	OLI	9.97E+06	2.31E+05	2.15E+06	1.24E+07
	TPENT2ENE	OLI	9.97E+06	2.31E+05	2.15E+06	1.24E+07
	PENT1ENE	OLT	3.52E+07	2.65E+05	6.81E+06	4.23E+07
	ME2BUT2ENE	OLI	1.14E+07	1.26E+05	2.66E+06	1.42E+07
	ME3BUT1ENE	OLT	1.44E+07	1.59E+05	3.36E+06	1.79E+07
	ME2BUT1ENE	OLI	2.14E+06	8.39E+04	4.11E+05	2.63E+06
Ethyne	C2H2	HC3	1.92E+09	3.11E+09	2.22E+09	7.25E+09

Table S4: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to RADM2 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	RADM2 Species	Belgium	Netherlands	Luxembourg	Total
Benzene	BENZENE	TOL	3.82E+09	8.93E+09	4.24E+09	1.70E+10
Toluene	TOLUENE	TOL	5.69E+09	1.21E+10	6.28E+09	2.41E+10
Xylenes	MXYL	XYL	1.71E+09	2.69E+09	1.69E+09	6.09E+09
	OXYL	XYL	7.74E+08	1.70E+09	8.68E+08	3.34E+09
	PXYL	XYL	7.44E+08	1.63E+09	8.16E+08	3.19E+09
Trimethylbenzenes	TM123B	XYL	4.54E+07	7.45E+07	5.23E+07	1.72E+08
	TM124B	XYL	1.77E+08	2.93E+08	2.45E+08	7.15E+08
	TM135B	XYL	5.64E+07	1.04E+08	7.19E+07	2.32E+08
Other Aromatics	EBENZ	TOL	4.50E+08	9.33E+08	7.08E+08	2.09E+09
	PBENZ	TOL	2.01E+08	5.86E+08	2.93E+08	1.08E+09
	IPBENZ	TOL	9.99E+07	1.32E+08	1.18E+08	3.50E+08
	PETHTOL	XYL	6.10E+07	1.06E+08	1.07E+08	2.74E+08
	METHTOL	XYL	7.00E+07	1.16E+08	1.14E+08	3.00E+08
	OETHTOL	XYL	4.24E+07	7.56E+07	7.71E+07	1.95E+08
	DIET35TOL	XYL	3.02E+08	1.04E+09	4.41E+08	1.78E+09
	DIME35EB	XYL	1.19E+08	2.11E+08	1.23E+08	4.53E+08
	STYRENE	TOL	7.61E+07	1.43E+08	1.29E+08	3.48E+08
	BENZAL	CSL	6.38E+07	2.20E+08	9.29E+07	3.77E+08
	PHENOL	CSL	1.69E+07	0.00E+00	4.81E+07	6.50E+07
Formaldehyde	HCHO	HCHO	2.35E+09	3.04E+09	3.38E+09	8.77E+09
Other Aldehydes	CH3CHO	ALD	4.61E+08	7.40E+08	4.46E+08	1.65E+09
	C2H5CHO	ALD	2.23E+08	2.46E+08	2.18E+08	6.87E+08
	C3H7CHO	ALD	1.98E+08	1.12E+08	1.76E+08	4.86E+08
	IPRCHO	ALD	1.60E+08	7.62E+07	1.34E+08	3.70E+08
	C4H9CHO	ALD	8.86E+07	5.10E+06	5.23E+07	1.46E+08
	ACR	ALD	1.39E+08	2.25E+08	1.22E+08	4.86E+08
	MACR	ALD	8.71E+07	5.02E+06	5.14E+07	1.44E+08
	C4ALDB	ALD	1.28E+08	1.62E+08	1.04E+08	3.94E+08
	MGLYOX	MGLY	4.52E+07	2.85E+07	3.36E+07	1.07E+08
Alkadienes and	C4H6	OLI	3.64E+10	1.12E+11	4.63E+10	1.95E+11
Other Alkynes	C5H8	ISO	3.35E+09	1.10E+10	0.00E+00	1.44E+10
Organic Acids	HCOOH	ORA1	9.28E+08	4.04E+07	4.74E+08	1.44E+09
	CH3CO2H	ORA2	7.55E+08	3.10E+07	4.88E+08	1.27E+09
	PROPACID	ORA2	8.65E+08	3.77E+07	4.42E+08	1.34E+09
	ACO2H	OLT	2.87E+07	0.00E+00	8.19E+07	1.11E+08

Table S4: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to RADM2 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	RADM2 Species	Belgium	Netherlands	Luxembourg	Total
Alcohols	CH3OH	HC3	7.59E+08	8.27E+08	6.37E+08	2.22E+09
	C2H5OH	HC3	2.27E+09	1.73E+09	1.78E+09	5.78E+09
	NPROPOL	HC5	1.29E+08	1.25E+08	9.70E+07	3.51E+08
	IPROPOL	HC5	1.92E+08	2.00E+08	1.54E+08	5.46E+08
	NBUTOL	HC8	9.67E+07	9.84E+07	7.55E+07	2.71E+08
	BUT2OL	HC8	7.14E+07	6.56E+07	5.17E+07	1.89E+08
	IBUTOL	HC8	4.54E+07	4.10E+07	3.15E+07	1.18E+08
	TBUTOL	HC3	2.40E+07	0.00E+00	1.24E+05	2.41E+07
	PECOH	HC8	9.27E+06	0.00E+00	4.77E+04	9.32E+06
	IPEAOH	HC8	9.27E+06	0.00E+00	4.77E+04	9.32E+06
	ME3BUOL	HC8	9.27E+06	0.00E+00	4.77E+04	9.32E+06
	IPECOH	HC3	2.53E+07	0.00E+00	1.30E+05	2.54E+07
	IPEBOH	HC8	9.27E+06	0.00E+00	4.77E+04	9.32E+06
	CYHEXOL	HC8	9.79E+06	0.00E+00	5.04E+04	9.84E+06
	MIBKAOH	KET	7.39E+07	6.36E+07	4.89E+07	1.86E+08
	ETHGLY	HC8	1.84E+07	1.47E+07	1.13E+07	4.44E+07
	PROPGLY	HC8	4.57E+07	4.39E+07	3.37E+07	1.23E+08
	C6H5CH2OH	HC8	2.64E+07	2.95E+07	2.26E+07	7.85E+07
	MBO	OLT	1.97E+07	0.00E+00	1.02E+05	1.98E+07
Ketones	CH3COCH3	KET	2.05E+09	2.11E+09	1.95E+09	6.11E+09
	MEK	KET	1.14E+09	1.23E+09	9.49E+08	3.32E+09
	MPRK	KET	1.03E+07	4.81E+05	4.23E+06	1.50E+07
	DIEK	KET	1.03E+07	4.81E+05	4.23E+06	1.50E+07
	MIPK	KET	1.03E+07	4.81E+05	4.23E+06	1.50E+07
	HEX2ONE	HC5	8.63E+06	4.03E+05	3.55E+06	1.26E+07
	HEX3ONE	HC5	8.63E+06	4.03E+05	3.55E+06	1.26E+07
	MIBK	HC5	8.34E+08	8.96E+08	6.95E+08	2.43E+09
	MTBK	KET	1.06E+07	4.96E+05	4.36E+06	1.55E+07
	CYHEXONE	HC5	8.73E+07	7.36E+07	9.18E+07	2.53E+08
Esters	METHACET	HC3	6.39E+07	0.00E+00	2.76E+06	6.67E+07
	ETHACET	HC3	2.04E+09	2.32E+09	1.78E+09	6.14E+09
	NBUTACET	HC5	1.29E+09	1.47E+09	1.13E+09	3.89E+09
	IPROACET	HC3	6.26E+08	7.14E+08	5.48E+08	1.89E+09
	CH3OCHO	HC3	1.19E+07	0.00E+00	5.16E+05	1.24E+07
	NPROACET	HC3	2.45E+08	2.68E+08	2.09E+08	7.22E+08

Table S4: Benelux AVOC and BVOC emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) mapped from MCMv3.2 species to RADM2 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2 Species	RADM2 Species	Belgium	Netherlands	Luxembourg	Total
Ethers	CH3OCH3	HC3	2.48E+08	6.41E+07	7.38E+07	3.86E+08
	DIETETHER	HC8	5.64E+07	7.40E+05	1.01E+07	6.72E+07
	MTBE	HC3	3.03E+07	2.12E+06	2.32E+07	5.56E+07
	DIIPREETHER	HC8	7.26E+07	8.06E+05	1.47E+07	8.81E+07
	ETBE	HC8	1.15E+07	8.06E+05	8.83E+06	2.11E+07
	MO2EOL	HC8	4.59E+07	4.22E+07	3.85E+07	1.27E+08
	EOX2EOL	HC8	5.16E+07	4.75E+07	4.33E+07	1.42E+08
	PR2OHMOX	HC8	9.46E+07	9.45E+07	8.00E+07	2.69E+08
	BUOX2ETOH	HC8	6.28E+08	6.76E+08	5.35E+08	1.84E+09
	BOX2PROL	HC8	1.04E+07	7.26E+05	7.97E+06	1.91E+07
Chlorinated Hydrocarbons	CH2CL2	HC3	2.87E+08	1.41E+08	3.53E+08	7.81E+08
	CH3CH2CL	HC3	9.35E+07	0.00E+00	2.66E+08	3.60E+08
	CH3CCL3	HC3	3.18E+08	1.97E+08	2.53E+08	7.68E+08
	TRICLETH	HC3	7.64E+08	4.45E+08	7.03E+08	1.91E+09
	CDICLETH	HC3	3.16E+07	0.00E+00	8.88E+07	1.20E+08
	TDICLETH	HC3	3.14E+07	0.00E+00	8.87E+07	1.20E+08
	CH3CL	HC3	4.78E+07	0.00E+00	1.36E+08	1.84E+08
	CCL2CH2	HC8	1.14E+07	0.00E+00	3.25E+07	4.39E+07
	CHCL2CH3	HC3	3.69E+05	0.00E+00	1.24E+05	4.93E+05
	VINCL	HC8	1.06E+07	0.00E+00	3.03E+07	4.09E+07
	TCE	HC3	1.82E+08	1.08E+08	1.60E+08	4.50E+08
	CHCL3	HC3	1.01E+07	0.00E+00	2.88E+07	3.89E+07
Terpenes	APINENE	OLI	8.78E+08	2.65E+09	3.05E+08	3.83E+09
	BPINENE	OLI	8.78E+08	2.65E+09	3.05E+08	3.83E+09
	LIMONENE	OLI	1.03E+09	2.80E+09	4.38E+08	4.27E+09
Total			5.83E+11	1.44E+12	6.42E+11	2.66E+12

Table S5: Benelux emissions (molecules $\text{cm}^{-2} \text{s}^{-1}$) of AVOC and BVOC species in CB05, determined by translating the MCMv3.2 emissions from Table S1 into CB05 species using Yarwood et al. (2005).

CB05 Species	Belgium	Luxembourg	Netherlands	Total
PAR	1.80E+12	4.90E+12	2.10E+12	8.80E+12
OLE	8.96E+10	2.70E+11	1.13E+11	4.73E+11
TOL	6.55E+09	1.39E+10	7.51E+09	2.80E+10
XYL	4.39E+09	8.50E+09	4.87E+09	1.78E+10
FORM	2.41E+09	3.09E+09	3.44E+09	8.94E+09
ALD2	5.64E+08	8.88E+08	5.37E+08	1.99E+09
ALDX	7.21E+08	6.35E+08	6.27E+08	1.98E+09
MEOH	2.20E+09	2.40E+09	1.85E+09	6.45E+09
ETOH	3.30E+09	2.51E+09	2.58E+09	8.39E+09
FACD	9.28E+08	4.04E+07	4.74E+08	1.44E+09
AACD	1.33E+09	5.61E+07	7.83E+08	2.17E+09
ETH	3.78E+10	7.68E+09	9.39E+09	5.49E+10
ETHA	4.91E+09	8.58E+08	7.96E+09	1.37E+10
IOLE	3.87E+07	4.43E+05	9.05E+06	4.82E+07
ISOP	3.35E+09	1.10E+10	0.00E+00	1.44E+10
TERP	1.34E+09	3.89E+09	5.03E+08	5.73E+09
Total	1.96E+12	5.23E+12	2.25E+12	9.44E+12

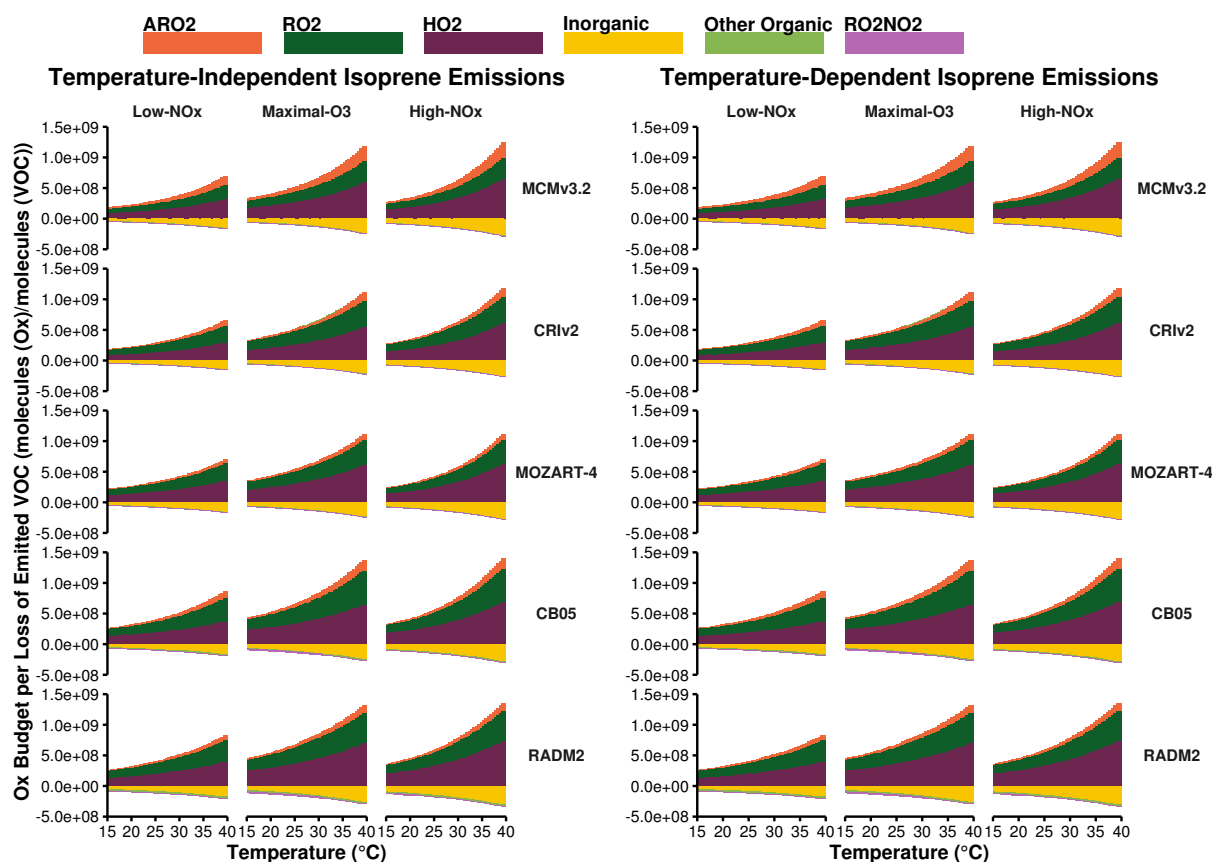
S3 Ozone Production and Consumption Budgets

Section 3.2 of the research article analysed the O_x production and consumption budgets normalised by the total loss rate of the emitted VOCs. The absolute O_x production and consumption budgets are included to support the conclusion that the increased OH-reactivity of the emitted VOCs caused the increase of ozone with temperature in our study. As in Fig. 4 of the research article the production and consumption of O_x are allocated to the net contributions of major categories: ‘ARO2’, ‘RO2’ and ‘HO2’ represent the reaction of acyl peroxy radicals, alkyl peroxy radicals and HO_2 with NO. ‘Inorganic’ represents the net contribution of inorganic reactions, ‘RO2NO2’ the net contribution of peroxy nitrates and any other reactions were allocated to the ‘Other Organic’ category. Figure S1a represents the absolute production and consumption budgets of O_x for each chemical mechanism, each NO_x -regime and using a temperature-independent and temperature-dependent source of isoprene emissions.

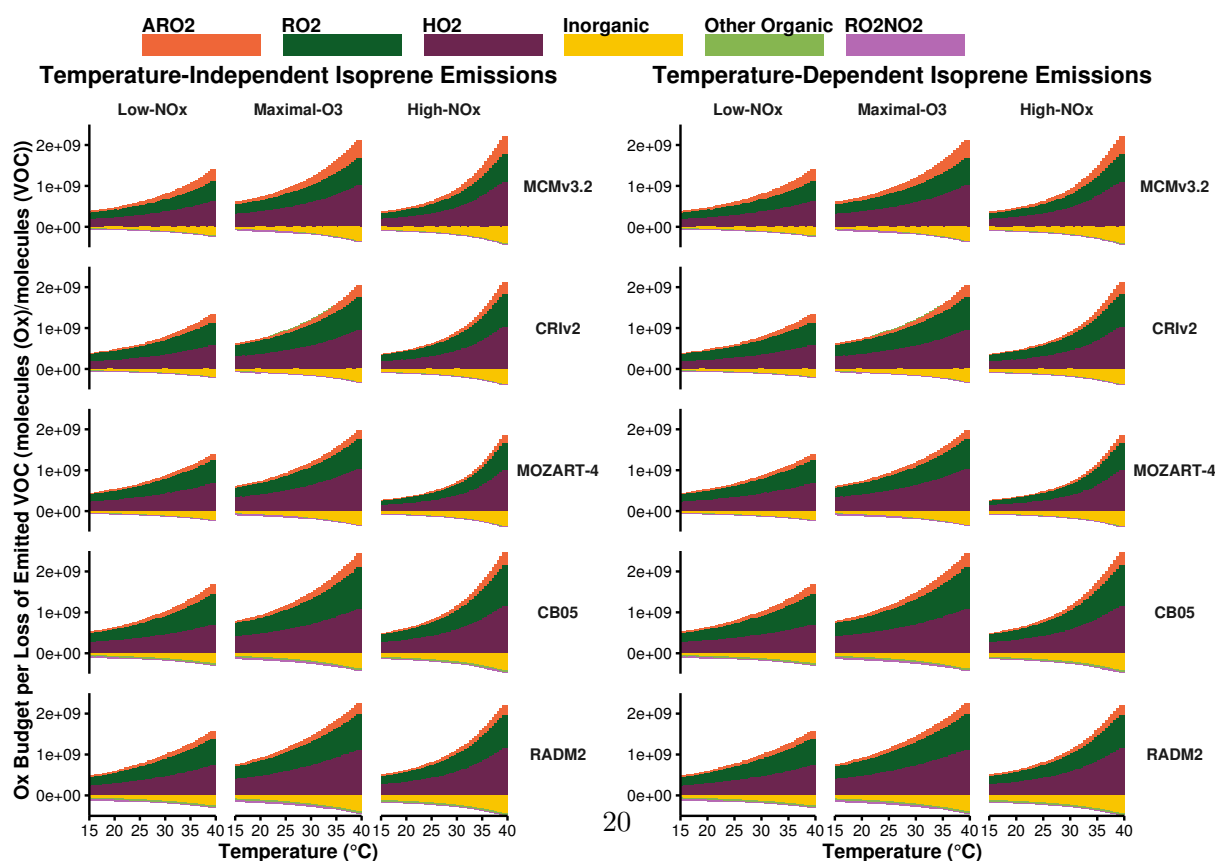
The absolute production and consumption budgets of O_x in the box model simulations without mixing, described in Section 3.3 of the research article, are illustrated in Fig. S1b. Similar to Fig. S1a, the increase in O_x with temperature is due to the increased OH-reactivity of emitted VOCs. The increased O_x with temperature led to the faster rate of increase in ozone with temperature than the original box model setup that included mixing, this is presented in Sect. 3.3 of the research article.

Figure S1: Day-time budgets of O_x allocated to the NO_x -regimes allocated to the net contribution of reactions to O_x budgets are allocated to categories of inorganic reactions, peroxy nitrates (RO2NO2), reactions of NO with HO2, alkyl peroxy radicals (RO2) and acyl peroxy radicals (ARO2). All other reactions are allocated to the 'Other Organic' category.

(a) O_x production and consumption budgets with box model setup including mixing.



(b) O_x production and consumption budgets with box model setup without including mixing.



References

- B. Bonn, E. von Schneidmesser, D. Andrich, J. Quedenau, H. Gerwig, A. Lüdecke, J. Kura, A. Pietsch, C. Ehlers, D. Klemp, C. Kofahl, R. Nothard, A. Kerschbaumer, W. Junkermann, R. Grote, T. Pohl, K. Weber, B. Lode, P. Schönberger, G. Churkina, T. M. Butler, and M. G. Lawrence. BAERLIN2014 - The influence of land surface types on and the horizontal heterogeneity of air pollutant levels in Berlin. *Atmospheric Chemistry and Physics Discussions*, 2016:1–62, 2016.
- J. Coates and T. M. Butler. A comparison of chemical mechanisms using tagged ozone production potential (TOPP) analysis. *Atmospheric Chemistry and Physics*, 15(15):8795–8808, 2015.
- J. J. P. Kuenen, A. J. H. Visschedijk, M. Jozwicka, and H. A. C. Denier van der Gon. TNO-MACC_II emission inventory; a multi-year (2003–2009) consistent high-resolution european emission inventory for air quality modelling. *Atmospheric Chemistry and Physics*, 14(20):10963–10976, 2014.
- A. S. M. Lourens, T. M. Butler, J. P. Beukes, P. G. van Zyl, G. D. Fourie, and M. G. Lawrence. Investigating atmospheric photochemistry in the Johannesburg-Pretoria megacity using a box model. *South African Journal of Science*, 112(1/2), 2016.
- G. Yarwood, S. Rao, M. Yocke, and G. Z. Whitten. Updates to the Carbon Bond Chemical Mechanism: CB05. Technical report, U. S Environmental Protection Agency, 2005.