- The Influence of Temperature on Ozone Production under
- varying NO_x Conditions a modelling study: Supplementary
- 3 Material
- J. Coates¹, K. A. Mar¹, N. Ojha² and T. M. Butler¹
- ¹Institute for Advanced Sustainability Studies, Potsdam, Germany
- ²Atmospheric Chemistry Department, Max Planck Institute for Chemistry, Mainz,
 - Germany

7

8

11

August 19, 2016

S1 Allocation of Benelux AVOC emissions to Mechanism Species

inventory (Kuenen et al., 2014) were translated to MCM v3.2 emissions (Table S1). The MCM v3.2 emissions for each initial species were translated to emissions of mechanism species into CRI v2, MOZART-4 and RADM2 chemical mechanisms by weighting with the carbon

Anthropogenic NMVOC emissions over Benelux specified by the TNO MACCIII emission

numbers (Tables S2 – S4). The allocation of MCM v3.2 emissions into CB05 species followed the

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	63860000		3.45e + 08	210200000		$1.3728e{+}10$
Propane	СЗН8	2.886e+09	1086600000	2.573e+09	1.041e+11	9.72e+08	47090000	202400000	038600000	62710000	249700000	75200000		1.129e + 11
D4	NC4H10	2.127e+09	882870000	949270000	6.11e+11	3.61e+09	1.048e + 09	209500000		1037800000	315300000	42200000		6.21e+11
Dutanes	IC4H10	258600000	309660000	232311000	1.486e + 11	163700000	489100000	97500000		483900000	157900000	42200000		1.509e + 11
	NC5H12	1.783e + 09	1014960000		4.548e + 11		6.27e + 08	8.4e+07		521500000	118200000	14890000		4.589e + 11
Pentanes	IC5H12	7.52e + 08	544340000		2.718e + 11		1.216e + 09	163500000		1011700000	225600000	14890000		2.762e + 11
	NEOP											14890000		14890000
	NC6H14	954100000	57390000	1.211e+09	6.49e+10	3.162e+09	2.207e+09	1.246e+09		193450000	4.26e+08	5160000		7.44e+10
	M2PE			156600000	9.98e + 09	6.66e + 08					7.08e + 08	2215000		1.151e+10
	M3PE			117100000	4.989e + 09	6.66e + 08					4.26e + 08			6.2e + 09
səu	NC7H16	409520000	98740000	5.71e+08	6.97e + 10	1.146e + 09	363500000	205300000		31790000	121900000	26040000		7.28e+10
rjksr	M2HEX					4.3e+08	2.83e + 08	159500000		24710000	182900000			1.08e + 09
√ 19	M3HEX					4.3e+08	2.02e + 08	1.14e + 08		17634000	121900000			8.86e+08
ńgi.	M22C4										141800000			141800000
ΗР	M23C4										141800000			141800000
une a	NC8H18			235300000	5.18e + 10	125600000	319500000	179700000		27890000	6.95e + 08	8900000		5.33e+10
сэпе	NC9H20			131200000		3.02e+09						2969000		3.148e + 09
кән	NC10H22			1.66e + 08		5.85e + 09	142200000	80300000		12458000		4460000		6.25e+09
	NC11H24			64600000		2.387e + 09	51830000	29280000		4536000	78100000	1625000		2.617e+09
	NC12H26					168500000	8.45e + 08	476900000		74100000	71700000			1.637e + 09
	CHEX		91490000	4e+07		6.82e+08						1506000		8.15e + 08
Ethene	C2H4	212300000	3695700000	3.368e + 10			5.341e + 09	3.807e + 09	342500000		4.62e+09	1.9e + 08		5.188e + 10
Propene	С3Н6	141700000	868200000	6.59e + 08			1.876e + 09	634800000	151810000		7.86e+08	54500000		5.18e + 09
	HEXIENE	21050000	15773000									21810000		58703000
	BUTIENE		22154000	240400000							24510000			286604000
	MEPROPENE										12260000			12260000
sət	TBUT2ENE										12260000			12260000
Ікет	CBUTZENE										12260000			12260000
A 1:	CPENT2ENE		6961000								4902000			11861000
эцзі	TPENT2ENE		6961000								4902000			11861000
!Н	PENT1ENE		6328000	6186000							19630000			32171000
	ME2BUT2ENE		3793000								0000086			13581000
	ME3BUT1ENE		3793000								0000086			13581000
	ME2BUT1ENE		2525500											2525500
Ethyne	C2H2	2697000	1252200000	426600000			4.975e + 09	1.795e + 09	134690000	252500000	1.614e + 09	71500000		$1.051e{+10}$
Benzene	GENTARINE	00000000000	1 000 - 000	00 - 0 0			11	00000000		000000000000000000000000000000000000000	-			

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).

C. a, 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	70200000	4880000		6.78e+09
Xylenes	OXYL	23330000	21179000	002699	1.994e + 09	9.84e + 08	5.77e + 08	61040000		4735000	57100000	2924000		3.717e + 09
	PXYL		21179000	002699	1.994e + 09	9.84e + 08	432900000	45800000		3551000	70200000	3909000		3.556e + 09
	TM123B	18550	1304500			6.6e+07	99200000				3330000	441000		170200000
Trimethylbenzenes	TM124B	18550	1304500	56100000		224600000	4.16e + 08				0000944	589000		7.06e + 08
	TM135B	18550	1304500			6.6e + 07	158600000				3330000	589000		229900000
	EBENZ	35100000		63400000		179400000	430600000	341600000	119530		8e+08	5250000		1.856e+09
	PBENZ					39600000	380600000	301500000	105570		128500000	2311000		8.53e + 08
	IPBENZ					145300000					128500000	2311000		276300000
sics	PETHTOL					13210000					257500000			270300000
mst	METHTOL					39600000					257500000			296300000
отА	OETHTOL										192800000			192800000
. Ter	DIET35TOL						8.05e + 08	637600000	223800					1.443e + 09
Ι [‡] Ο	DIME35EB					224700000	99300000	78700000	27540					4.03e + 08
	STYRENE			64600000		45700000	91500000	72500000	25440					275100000
	BENZAL						153900000	121900000	42690					275900000
	PHENOL			71500000										71500000
Formaldehyde	нсно	611400000	2195300000				1.177e + 09	1.781e+09	85260000		2.9e+09	29490000		8.77e+09
	СНЗСНО	11780000	130090000	73750000			318400000	7.39e + 08	16383000		6.8e + 08	0000989		1.976e + 09
	C2H5CHO	6710000	98630000				53670000	124600000	2752000		257700000	5200000		5.49e + 08
səp	C3H7CHO	38630	79420000								207600000	4190000		292100000
бүә	IPRCHO	38630	79420000								138400000	4190000		222100000
ΡΙΨ	C4H9CHO	32340	66550000									3504000		70050000
рег	ACR	49770	102260000				83300000	193800000	4282000			5390000		388800000
[1 O	MACR	39730	81710000									4310000		86110000
	C4ALDB	39730	81710000				44510000	103300000	2287000			4310000		236100000
	MGLYOX										138500000			138500000
Alkadienes and	C4H6	00000929	771300000	4.74e+09	2.221e + 11		2.505e + 09	7.78e+08	245800000	458800000	1.033e+09	52800000		2.332e + 11
Other Alkynes	C5H8												1.435e + 10	1.435e+10
	нсоон	4660000	1201400000								1.67e + 08	69400000		1442400000
Organia Acida	СНЗСО2Н	3572000	9.21e + 08	167700000							$1.28\mathrm{e}\!+\!08$	53200000		1.274e + 09
Seminary Company	PROPACID	2898000	746100000								1.04e + 08	43100000		897100000
	ACO2H			140400000										140400000

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
	СНЗОН	140000		3200000		6.38e+09					40419000	24020000		6.45e + 09
	С2Н5ОН	97400	1.687e + 09	90300000		6.52e + 09					28082900	63300000		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
slo	PECOH	50900									14643300			14775400
оцоз	IPEAOH	50900									14643300			14775400
ρΙΨ	ME3BUOL	50900									14643300			14775400
	IPECOH	50900									14643300			14775400
	ІРЕВОН	20900									14643300			14775400
	CYHEXOL	44800									12938100			12966400
	MIBKAOH	38600				109900000					11132900			121100000
	ETHGLY	72300				154300000					20861500			175200000
	PROPGLY	59000				307800000					16950200			324800000
	С6Н5СН2ОН					88500000								88500000
	MBO	52100									15044300			15077200
	СНЗСОСНЗ	384100	15896000	6.38e + 08		60 + 999.9	35750000	229900000			382100000	1414000		7.96e+09
	MEK		12828000			3.212e+09						1139000		3.236e + 09
	MPRK		10745000									954000		11705000
S	DIEK		10745000									954000		11705000
səuo	MIPK		10745000									954000		11705000
одәу	HEX2ONE		9242000									820000		10062000
I	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
Terpenes	BPINENE											3050000	1.835e + 09	1.839e + 09
	LIMONENE					209500000						4580000	1.835e + 09	2.046e + 09
	METHACET			64470000										64470000
	ETHACET			7386000		4.44e+09								4.45e+09
SIO	NBUTACET					3.113e + 09								3.113e + 09
ısı	IPROACET					1.095e + 09								1.095e + 09

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).

Cu ai., 2017).	1.													
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
	СНЗОСНО			7229000										7229000
	NPROACET					4.1e+08						7950000		4.18e + 08
	СНЗОСНЗ		61750000	253500000		244300000								5.59e+08
	DIETETHER		38360000	94510000										132360000
	MTBE		32330000											32330000
	DIIPRETHER		27860000	68540000								19520000		115960000
ers.	ETBE		27860000											27860000
मभ्ञ	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
suc	CH3CCL3					1.113e + 09						464000		1.114e + 09
ирс	TRICLETH			256600000		2.516e + 09						471000		2.776e + 09
:00:	CDICLETH			173100000								951000		174800000
ΡΛΉ	TDICLETH			173100000								634000		174600000
I þə	CH3CL			5.34e + 08										5.34e + 08
oten	CCL2CH2			173100000										173100000
irol.	CHCL2CH3											715000		715000
СР	VINCL			1.62e + 08										1.62e + 08
	TCE			40500000		6.11e + 08						927000		6.53e + 08
	CHCL3			112800000										112800000
T.	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 $\rm cm^{-2}~s^{-1}$) mapped from MCMv3.2 species to CRIv2 species by weighting with the carbon numbers of the respective species.

Trumo	MCMv3.2	CRIv2	Belgium	Nothonlondo	Turromborra	Total
Type	Species	Species	Deigium	Netherlands	Luxembourg	Total
Ethane	C2H6	C2H6	4.91E+09	8.58E+08	7.96E+09	1.37E + 10
Propane	С3Н8	С3Н8	3.35E+10	4.00E+10	3.94E+10	1.13E+11
Darkanaa	NC4H10	NC4H10	1.25E+11	3.49E+11	1.47E+11	6.21E+11
Butanes	IC4H10	IC4H10	$3.03E{+}10$	$8.50E{+}10$	$3.56E{+}10$	$1.51E{+}11$
	NC5H12	NC5H12	8.89E+10	2.65E+11	1.05E+11	4.59E+11
Pentanes	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
	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
ω	NC7H16	NC7H16	$1.45E{+}10$	4.12E + 10	1.71E+10	7.28E+10
Hexane and Higher Alkanes	M2HEX	M2HEX	2.74E + 08	4.89E + 08	3.17E + 08	1.08E+09
r All	M3HEX	M3HEX	2.37E + 08	3.90E + 08	2.59E+08	8.86E + 08
lighe	M22C4	M22C4	3.47E + 07	5.29E+07	5.42E+07	1.42E+08
H pu	M23C4	M23C4	3.47E + 07	5.29E+07	5.42E+07	1.42E + 08
ne a	NC8H18	NC8H18	$1.04E{+}10$	$3.06E{+}10$	1.23E+10	5.33E+10
Hexa	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
Ethene Propene	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
	C2H4	C2H4	$3.66E{+}10$	7.03E+09	8.25E+09	5.19E+10
	С3Н6	С3Н6	1.82E+09	1.68E+09	1.68E+09	5.18E+09
	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
δ.	TBUT2ENE	TBUT2ENE	9.80E + 06	0.00E+00	2.46E+06	1.23E+07
Higher Alkenes	CBUT2ENE	CBUT2ENE	9.80E + 06	0.00E+00	2.46E+06	1.23E+07
er Al	CPENT2ENE	CPENT2ENE	9.57E + 06	2.21E + 05	2.07E+06	1.19E+07
lighe	TPENT2ENE	TPENT2ENE	9.57E + 06	2.21E + 05	2.07E + 06	1.19E+07
<u> </u>	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 $\rm cm^{-2}~s^{-1}$) mapped from MCMv3.2 species to CRIv2 species by weighting with the carbon numbers of the respective species.

Typo	MCMv3.2	CRIv2	Boloi	Netherlands	Luxembaue	Total
Type	Species	Species	Belgium	retherlands	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
	MXYL	MXYL	1.90E+09	3.00E+09	1.88E+09	6.78E + 09
Xylenes	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
	TM123B	TM123B	4.49E+07	7.36E+07	5.17E+07	1.70E + 08
Trimethylbenzenes	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
	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
S	PETHTOL	PETHTOL	6.03E+07	1.05E + 08	1.05E+08	2.70E + 08
mati	METHTOL	METHTOL	6.93E + 07	1.14E + 08	1.13E+08	2.96E + 08
Other Aromatics	OETHTOL	OETHTOL	4.19E + 07	7.47E + 07	7.62E + 07	1.93E+08
ther	DIET35TOL	DIET35TOL	2.45E + 08	8.42E + 08	3.56E + 08	1.44E+09
Ó	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	НСНО	НСНО	2.35E+09	3.04E+09	3.38E+09	8.77E+09
	СНЗСНО	СНЗСНО	5.53E+08	8.88E+08	5.35E + 08	1.98E+09
	С2Н5СНО	С2Н5СНО	1.78E + 08	1.97E + 08	1.74E + 08	5.49E + 08
S	СЗН7СНО	СЗН7СНО	1.19E + 08	6.71E + 07	1.06E + 08	2.92E + 08
Other Aldehydes	IPRCHO	IPRCHO	9.60E + 07	4.57E + 07	8.04E + 07	2.22E + 08
Alde	С4Н9СНО	С4Н9СНО	4.25E + 07	2.45E + 06	2.51E+07	7.01E+07
ther	ACR	UCARB10	8.33E+07	1.35E + 08	7.33E+07	2.92E + 08
0	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
	НСООН	НСООН	9.28E+08	4.04E+07	4.74E+08	1.44E+09
0	СН3СО2Н	СН3СО2Н	7.55E+08	3.10E + 07	4.88E + 08	1.27E+09
Organic Acids	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 $\rm cm^{-2}~s^{-1}$) mapped from MCMv3.2 species to CRIv2 species by weighting with the carbon numbers of the respective species.

Trung	MCMv3.2	CRIv2	Belgium	Netherlands	Luxembourg	Total
Type	Species	Species	Deigium	Netherlands	Luxembourg	Total
	СНЗОН	СНЗОН	2.20E+09	2.40E+09	1.85E+09	6.45E + 09
	С2Н5ОН	С2Н5ОН	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
slo	PECOH	PECOH	1.47E + 07	0.00E+00	7.54E + 04	1.48E + 07
Alcohols	IPEAOH	IPEAOH	1.47E + 07	0.00E+00	7.54E + 04	1.48E + 07
A	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
	С6Н5СН2ОН	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	СНЗСОСНЗ	СНЗСОСНЗ	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
	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
ers	NBUTACET	NBUTACET	1.03E+09	1.18E + 09	9.03E + 08	3.11E+09
Esters	IPROACET	IPROACET	3.63E + 08	4.14E + 08	3.18E + 08	1.10E+09
	СНЗОСНО	СНЗОСНО	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 $\rm cm^{-2}~s^{-1}$) mapped from MCMv3.2 species to CRIv2 species by weighting with the carbon numbers of the respective species.

	MCMv3.2	CRIv2				
\mathbf{Type}	Species	Species	Belgium	Netherlands	Luxembourg	Total
	СНЗОСНЗ	СНЗОСНЗ	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
	DIIPRETHER	DIIPRETHER	9.56E + 07	1.06E + 06	1.93E+07	1.16E + 08
Ethers	ETBE	ETBE	1.52E + 07	1.06E + 06	1.16E + 07	2.79E+07
Eth	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
	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
pons	TRICLETH	C2H4	1.11E+09	6.46E + 08	1.02E + 09	2.78E+09
ocar	CDICLETH	C2H4	4.58E + 07	0.00E+00	1.29E + 08	1.75E + 08
Chlorinated Hydrocarbons	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
rina	CCL2CH2	C2H4	4.51E+07	0.00E+00	1.28E + 08	1.73E + 08
Chlo	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
	APINENE	APINENE	4.22E+08	1.27E+09	1.47E + 08	1.84E+09
Terpenes	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
Tot	al		5.15E+11	1.25E+12	5.64E+11	2.32E+12

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

Tuno	MCMv3.2	MOZART-4	Dolo-!	No. 4 la a 1 1	T	Total
Type	Species	Species	Belgium	Netherlands	Luxembourg	Iotai
Ethane	С2Н6	C2H6	4.91E+09	8.58E+08	7.96E+09	1.37E+10
Propane	СЗН8	СЗН8	3.35E+10	4.00E+10	3.94E+10	1.13E+11
D. /	NC4H10	BIGALK	1.00E+11	2.79E+11	1.17E+11	4.96E+11
Butanes	IC4H10	BIGALK	2.42E+10	6.80E + 10	2.85E + 10	1.21E+11
	NC5H12	BIGALK	8.89E+10	2.65E+11	1.05E+11	4.59E+11
Pentanes	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
	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
ro.	NC7H16	BIGALK	2.02E+10	5.77E + 10	2.39E+10	1.02E+11
kanek	M2HEX	BIGALK	3.83E + 08	6.84E + 08	4.44E + 08	1.51E+09
r All	M3HEX	BIGALK	3.31E + 08	5.45E + 08	3.63E + 08	1.24E+09
ighe	M22C4	BIGALK	4.16E + 07	6.34E + 07	6.51E + 07	1.70E+08
H pu	M23C4	BIGALK	4.16E + 07	6.34E + 07	6.51E + 07	1.70E + 08
ne aı	NC8H18	BIGALK	1.67E + 10	4.89E + 10	1.97E + 10	8.53E+10
Hexane and Higher Alkanes	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
Ethene	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	С3Н6	С3Н6	1.82E+09	1.68E+09	1.68E+09	5.18E+09
	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+0'
∞	TBUT2ENE	BIGENE	9.80E + 06	0.00E+00	2.46E + 06	1.23E+0
kene	CBUT2ENE	BIGENE	9.80E + 06	0.00E+00	2.46E + 06	1.23E+0'
Higher Alkenes	CPENT2ENE	BIGENE	1.20E + 07	2.77E + 05	2.58E + 06	1.49E+0
lighe	TPENT2ENE	BIGENE	1.20E + 07	2.77E + 05	2.58E + 06	1.49E+0'
<u> </u>	PENT1ENE	BIGENE	3.34E+07	2.52E + 05	6.47E + 06	4.01E+0'
	ME2BUT2ENE	BIGENE	1.37E+07	1.51E + 05	3.20E + 06	1.71E+0
	ME3BUT1ENE	BIGENE	1.37E+07	1.51E + 05	3.20E+06	1.71E+0
	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 $\rm cm^{-2}~s^{-1}$) mapped from MCMv3.2 species to MOZART-4 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2	MOZART-4	Roleium	Netherlands	Luvomboura	Total
Type	Species	Species	Belgium	rvetherlands	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
	MXYL	TOLUENE	2.17E+09	3.43E+09	2.14E+09	7.74E+09
Xylenes	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
	TM123B	TOLUENE	5.78E + 07	9.47E + 07	6.65E+07	2.19E+08
Trimethylbenzenes	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
	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
S	PETHTOL	TOLUENE	7.76E+07	1.34E + 08	1.36E + 08	3.48E+08
Other Aromatics	METHTOL	TOLUENE	8.90E+07	1.47E + 08	1.45E+08	3.81E+08
Aroı	OETHTOL	TOLUENE	5.39E+07	9.61E + 07	9.80E + 07	2.48E+08
ther	DIET35TOL	TOLUENE	3.84E + 08	1.32E + 09	5.60E + 08	2.26E+09
Ö	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	НСНО	CH2O	2.35E+09	3.04E+09	3.38E+09	8.77E+09
	СНЗСНО	СНЗСНО	5.53E+08	8.88E+08	5.35E+08	1.98E+09
	С2Н5СНО	СНЗСНО	2.67E + 08	2.95E + 08	2.61E+08	8.23E+08
S	СЗН7СНО	СНЗСНО	2.37E + 08	1.34E + 08	2.11E+08	5.82E + 08
ehyd.	IPRCHO	СНЗСНО	1.92E + 08	9.14E + 07	1.61E+08	4.44E+08
Alde	С4Н9СНО	СНЗСНО	1.06E + 08	6.13E + 06	6.27E + 07	1.75E + 08
Other Aldehydes	ACR	MACR	8.33E+07	1.35E + 08	7.33E+07	2.92E+08
0	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	СНЗСОСНО	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
	НСООН	НСООН	9.28E+08	4.04E+07	4.74E+08	1.44E+09
			7 5 5 5 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	2.10E+07	4 00E + 00	1.27E+09
0	CH3CO2H	СНЗСООН	7.55E + 08	3.10E + 07	4.88E + 08	1.211 03
Organic Acids	CH3CO2H PROPACID	СНЗСООН	7.55E+08 8.65E+08	3.77E+07	4.42E+08	1.34E+09

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

Type	MCMv3.2	MOZART-4	Doloi	Notherland-	Luvombour	Total
Type	Species	Species	Belgium	Netherlands	Luxembourg	Total
	СНЗОН	СНЗОН	2.20E+09	2.40E+09	1.85E+09	6.45E+09
	С2Н5ОН	С2Н5ОН	3.30E+09	2.51E+09	2.58E + 09	8.39E+09
	NPROPOL	С2Н5ОН	3.08E + 08	3.00E + 08	2.33E+08	8.41E+08
	IPROPOL	С2Н5ОН	4.61E + 08	4.79E + 08	3.69E + 08	1.31E+09
	NBUTOL	С2Н5ОН	3.82E + 08	3.89E + 08	2.98E + 08	1.07E+09
	BUT2OL	С2Н5ОН	2.82E + 08	2.59E + 08	2.04E+08	7.45E+08
	IBUTOL	С2Н5ОН	1.79E + 08	1.62E + 08	1.24E + 08	4.65E+08
	TBUTOL	С2Н5ОН	3.48E + 07	0.00E+00	1.79E + 05	3.50E+07
slo	PECOH	С2Н5ОН	3.66E + 07	0.00E+00	1.88E + 05	3.68E+07
Alcohols	IPEAOH	С2Н5ОН	3.66E + 07	0.00E+00	1.88E + 05	3.68E+07
A	ME3BUOL	С2Н5ОН	3.66E + 07	0.00E+00	1.88E + 05	3.68E+07
	IPECOH	С2Н5ОН	3.66E + 07	0.00E+00	1.88E + 05	3.68E+07
	IPEBOH	С2Н5ОН	3.66E + 07	0.00E+00	1.88E + 05	3.68E+07
	CYHEXOL	С2Н5ОН	3.87E + 07	0.00E+00	1.99E + 05	3.89E+07
	MIBKAOH	С2Н5ОН	1.44E + 08	1.24E + 08	9.53E + 07	3.63E+08
	ETHGLY	С2Н5ОН	7.26E + 07	5.80E + 07	4.46E + 07	1.75E+08
	PROPGLY	С2Н5ОН	1.80E + 08	1.73E + 08	1.33E+08	4.86E+08
	С6Н5СН2ОН	С2Н5ОН	1.04E + 08	1.17E + 08	8.94E + 07	3.10E + 08
	MBO	С2Н5ОН	3.75E + 07	0.00E+00	1.93E + 05	3.77E+07
	СНЗСОСНЗ	СНЗСОСНЗ	2.67E + 09	2.75E+09	2.54E+09	7.96E+09
nes	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
Ketones	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
	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
ers	NBUTACET	BIGALK	1.24E+09	1.41E+09	5.15E+07	2.70E+09
Esters	IPROACET	BIGALK	3.63E + 08	4.14E + 08	7.90E+07	8.56E+08
	СНЗОСНО	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 $\rm cm^{-2}~s^{-1}$) mapped from MCMv3.2 species to MOZART-4 species by weighting with the carbon numbers of the respective species.

	MCMv3.2	MOZART-4	D.1.	NT 41 1 1	т 1	m . 1
Type	Species	Species	Belgium	Netherlands	Luxembourg	Total
	СНЗОСНЗ	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
	DIIPRETHER	BIGALK	1.15E + 08	1.27E + 06	1.60E + 06	1.18E + 08
Ethers	ETBE	BIGALK	1.82E + 07	1.27E + 06	1.03E+09	1.05E+09
Eth	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
	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
bons	TRICLETH	BIGALK	4.43E + 08	2.58E + 08	1.40E+07	7.15E + 08
ocar	CDICLETH	BIGALK	1.83E + 07	0.00E+00	6.08E + 07	7.91E+07
Chlorinated Hydrocarbons	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
rina	CCL2CH2	BIGALK	1.80E + 07	0.00E+00	8.46E + 08	8.64E + 08
Chlc	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
	APINENE	C10H16	4.22E + 08	1.27E + 09	4.78E + 07	1.74E + 09
Terpenes	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
Tot	al		$5.05E{+}11$	1.21E+12	5.39E+11	$2.25E{+}12$

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

Туре	MCMv3.2	RADM2	-	Netherlands	T 1	
	Species	Species	Belgium		Luxembourg	Total
Ethane	С2Н6	ETH	4.91E+09	8.58E+08	7.96E+09	1.37E+10
Propane	С3Н8	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
	NC5H12	HC5	9.26E+10	2.76E+11	1.09E+11	4.78E+11
Pentanes	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
	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
10	NC7H16	HC5	2.11E+10	6.01E + 10	2.49E+10	1.06E + 11
sanes	M2HEX	HC8	2.42E + 08	4.33E + 08	2.81E + 08	9.56E + 08
Hexane and Higher Alkanes	M3HEX	HC8	2.10E+08	3.45E + 08	2.30E + 08	7.85E+08
ighe	M22C4	HC3	7.18E + 07	1.09E + 08	1.12E + 08	2.93E + 08
н рг	M23C4	HC5	4.34E+07	6.61E + 07	6.78E + 07	1.77E + 08
ne aı	NC8H18	HC8	1.06E + 10	3.10E + 10	1.25E+10	5.41E+10
Iexa	NC9H20	HC8	1.26E+09	1.22E+09	1.11E+09	3.59E+09
н	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	СЗН6	OLT	1.43E+09	1.32E+09	1.32E+09	4.07E+09
	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
Higher Alkenes	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	НС3	1.92E+09	3.11E+09	2.22E+09	7.25E+09

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

Type	MCMv3.2	RADM2	Belgium	Netherlands	Luxembourg	Total
Туре	Species	Species	Beigium			
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
	MXYL	XYL	1.71E+09	2.69E+09	1.69E+09	6.09E+09
Xylenes	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
	TM123B	XYL	4.54E+07	7.45E+07	5.23E+07	1.72E+08
Trimethylbenzenes	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
	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
SS	PETHTOL	XYL	6.10E + 07	1.06E + 08	1.07E + 08	2.74E+08
Other Aromatics	METHTOL	XYL	7.00E+07	1.16E + 08	1.14E + 08	3.00E+08
Aroi	OETHTOL	XYL	4.24E+07	7.56E + 07	7.71E+07	1.95E+08
ther	DIET35TOL	XYL	3.02E + 08	1.04E+09	4.41E + 08	1.78E+09
Ö	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	НСНО	НСНО	2.35E+09	3.04E+09	3.38E+09	8.77E+09
	СНЗСНО	ALD	4.61E+08	7.40E+08	4.46E+08	1.65E+09
	С2Н5СНО	ALD	2.23E+08	2.46E + 08	2.18E + 08	6.87E + 08
Sea	СЗН7СНО	ALD	1.98E + 08	1.12E + 08	1.76E + 08	4.86E + 08
ehyd	IPRCHO	ALD	1.60E + 08	7.62E + 07	1.34E + 08	3.70E + 08
Alde	С4Н9СНО	ALD	8.86E + 07	5.10E + 06	5.23E+07	1.46E + 08
Other Aldehydes	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
	НСООН	ORA1	9.28E+08	4.04E+07	4.74E+08	1.44E+09
0	СН3СО2Н	ORA2	7.55E+08	3.10E+07	4.88E + 08	1.27E+09
Organic Acids	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 $\rm cm^{-2}~s^{-1}$) mapped from MCMv3.2 species to RADM2 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2	RADM2	D.1.	NT /1 1 1	т 1	
	Species	Species	Belgium	Netherlands	Luxembourg	Total
	СНЗОН	HC3	7.59E+08	8.27E+08	6.37E+08	2.22E+09
	С2Н5ОН	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
ols	PECOH	HC8	9.27E + 06	0.00E+00	4.77E + 04	9.32E + 06
Alcohols	IPEAOH	HC8	9.27E + 06	0.00E+00	4.77E + 04	9.32E + 06
A	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
	С6Н5СН2ОН	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
	СНЗСОСНЗ	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
Ketones	MIPK	KET	1.03E+07	4.81E + 05	4.23E+06	1.50E + 07
Keto	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
	СНЗОСНО	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 $\rm cm^{-2}~s^{-1}$) mapped from MCMv3.2 species to RADM2 species by weighting with the carbon numbers of the respective species.

Type	MCMv3.2	RADM2	Belgium	Netherlands	Luxembourg	Total
	Species	Species				
	СНЗОСНЗ	НС3	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
	DIIPRETHER	HC8	7.26E + 07	8.06E + 05	1.47E + 07	8.81E + 07
Ethers	ETBE	HC8	1.15E+07	8.06E + 05	8.83E + 06	2.11E+07
Eth	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
	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
Chlorinated Hydrocarbons	TRICLETH	HC3	7.64E + 08	4.45E + 08	7.03E+08	1.91E + 09
ocar	CDICLETH	HC3	3.16E + 07	0.00E+00	8.88E + 07	1.20E + 08
Hydr	TDICLETH	HC3	$3.14\mathrm{E}{+07}$	0.00E+00	8.87E + 07	1.20E + 08
ted l	CH3CL	HC3	4.78E + 07	0.00E + 00	1.36E + 08	1.84E + 08
orina	CCL2CH2	HC8	$1.14\mathrm{E}{+07}$	0.00E+00	3.25E + 07	4.39E+07
Chlc	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
	APINENE	OLI	8.78E + 08	2.65E + 09	3.05E+08	3.83E+09
Terpenes	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 $\rm cm^{-2}~s^{-1}$) 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

S2 Extra Plots

Figure S1: NO_x emissions required for each chemical mechanism to achieve maximal ozone production at each temperature when using a temperature-independent and temperature-dependent source of isoprene emissions.

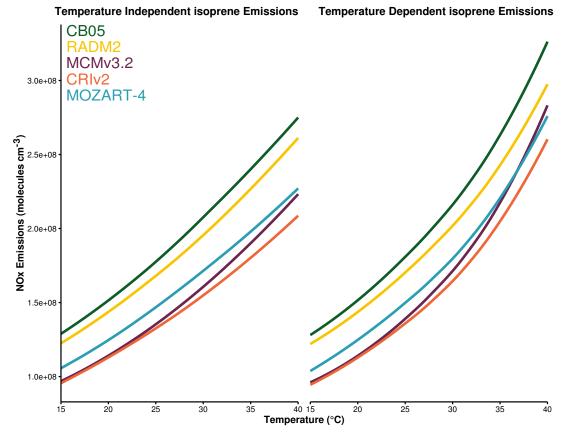
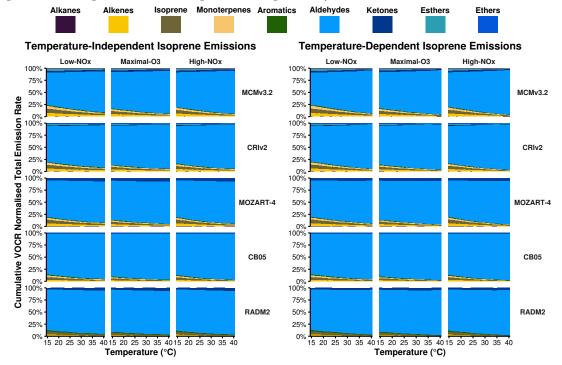


Figure S2: Contributions to cumulative VOC reactivity (VOCR) from different functional groups of emitted VOCs to the total VOCR. The contributions are normalised by the emissions of each VOC to illustrate the reactivity of each category per molecule emitted. Results illustrated at each temperature, for each chemical mechanism and source of isoprene emissions (temperature-independent and temperature-dependent).

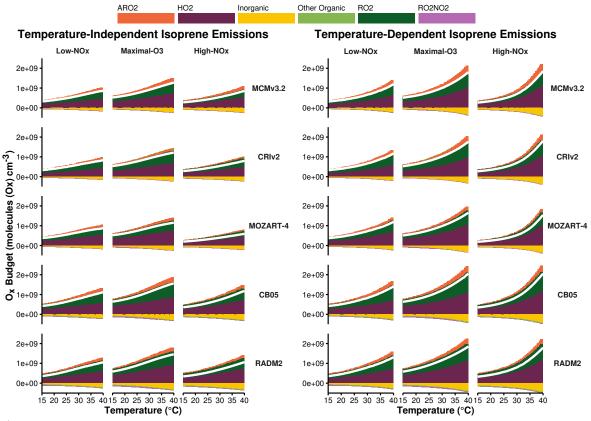


18 S3 Ox Production and Consumption Budgets

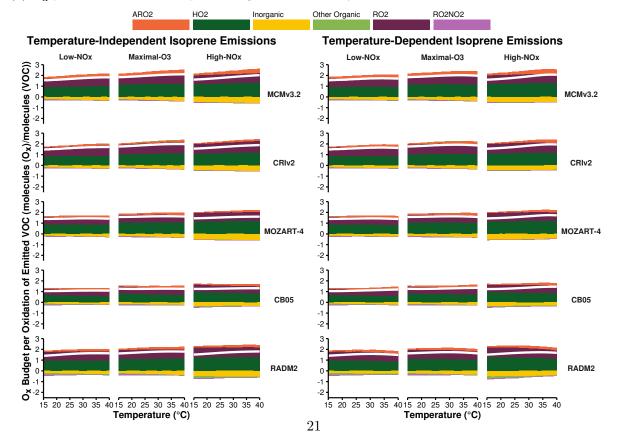
Further box model simulations of stagnant conditions were performed as outlined in Section 3.3 19 of the research article and an analysis similar to that Section 3.2 of the research article looked at 20 the production and consumption budgets of O_x was performed. As in Fig. 4 of the research article 21 the production and consumption of O_x are allocated to the net contributions of major categories: 22 'ARO2', 'RO2' and 'HO2' represent the reaction of acyl peroxy radicals, alkyl peroxy radicals 23 and HO₂ with NO. 'Inorganic' represents the net contribution of inorganic reactions, 'RO2NO2' 24 the net contribution of peroxy nitrates and any other reactions were allocated to the 'Other Organic' category. The absolute O_x production and consumption budgets for these addition simulations are depicted in Fig. S3a while the O_x budgets normalised by the total chemical 27 loss rate of emitted VOC are displayed in Fig. S3b. These O_x budgets are displayed for each 28 chemical mechanism, NO_x condition and source of isoprene emissions (temperature independent 29 and temperature dependent) in Figs. S3a and S3b. This analysis support the conclusion that the 30 increased OH-reactivity of the emitted VOCs caused the increase of ozone with temperature in our study.

Figure S3: Day-time budgets of O_x from box model simulations without mixing 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) Absolute O_x production and consumption budgets.



(b) O_x production and consumption budgets normalised by the total chemical loss rate of emitted VOC.



References

- 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):
- 37 10963–10976, 2014.
- ³⁸ 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.