

# The Influence of Temperature on Ozone Production under varying NO<sub>x</sub> Conditions – a modelling study: Supplementary Material

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## **S1 Allocation of Benelux AVOC emissions to Mechanism Species**

Anthropogenic NMVOC emissions over Benelux specified by the TNO\_MACCIII emission 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 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  $\text{cm}^{-2} \text{s}^{-1}$ ) 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      |
|---------------------------|-------------|------------|------------|------------|-----------|------------|------------|------------|------------|-------------|------------|-----------|------|------------|
| 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 | 987400000  | 5.71e+08   | 6.97e+10  | 1.146e+09  | 3635000000 | 2053000000 |            | 317900000   | 1219000000 | 260400000 |      | 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        |            |            | 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    |            |            |            |           |            |            |            |            |             |            |           |      | 122600000  |
|                           | CBUT2ENE    |            |            |            |           |            |            |            |            |             |            |           |      | 122600000  |
|                           | CPENT2ENE   |            | 6961000    |            |           |            |            |            |            |             |            |           |      | 118610000  |
|                           | TPENT2ENE   |            | 6961000    |            |           |            |            |            |            |             |            |           |      | 118610000  |
|                           | PENT1ENE    |            | 6328000    | 6186000    |           |            |            |            |            |             |            |           |      | 321710000  |
|                           | ME2BUT2ENE  |            | 3793000    |            |           |            |            |            |            |             |            |           |      | 135810000  |
|                           | ME3BUT1ENE  |            | 3793000    |            |           |            |            |            |            |             |            |           |      | 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    |           |            |           |           | 224700000  | 99300000  | 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  |

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| 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  |           |           |        |           | 109900000 |           |         | 11132900  |           |         |           | 121100000 |
|          | ETHGLY      | 72300  |           |           |        | 154300000 |           |           |         | 20861500  |           |         |           | 175200000 |
|          | PROPGLY     | 59000  |           |           |        | 307800000 |           |           |         | 16950200  |           |         |           | 324800000 |
|          | C6H5CH2OH   |        |           |           |        | 88500000  |           |           |         |           |           |         |           | 88500000  |
| Ketones  | MBO         | 52100  |           |           |        |           |           |           |         | 15044300  |           |         |           | 15077200  |
|          | 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 |
| Terpenes | 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 |

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|--------------------------|-------------|-----------|------------|----------|-----------|-----------|----------|-----------|------------|-----------|-----------|-----------|------------|-----------|
| 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  |
|                          | CH3CCL3     |           |            |          |           | 1.113e+09 |          |           |            |           | 464000    |           |            | 1.114e+09 |
| Chlorinated Hydrocarbons | 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<br>Species | CRIv2<br>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<br>Species | CRIv2<br>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<br>Species | CRIv2<br>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 |
| Ketones  | 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 |
|          | 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<br>Species | CRIv2<br>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<br>Species | MOZART-4<br>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<sup>-2</sup> s<sup>-1</sup>) mapped from MCMv3.2 species to MOZART-4 species by weighting with the carbon numbers of the respective species.

| Type              | MCMv3.2<br>Species | MOZART-4<br>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<br>Species | MOZART-4<br>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 cm<sup>-2</sup> s<sup>-1</sup>) mapped from MCMv3.2 species to MOZART-4 species by weighting with the carbon numbers of the respective species.

| Type                     | MCMv3.2<br>Species | MOZART-4<br>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<br>Species | RADM2<br>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<br>Species | RADM2<br>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<br>Species | RADM2<br>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<br>Species | RADM2<br>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 |

## 17 S2 Extra Plots

Figure S1:  $\text{NO}_x$  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.

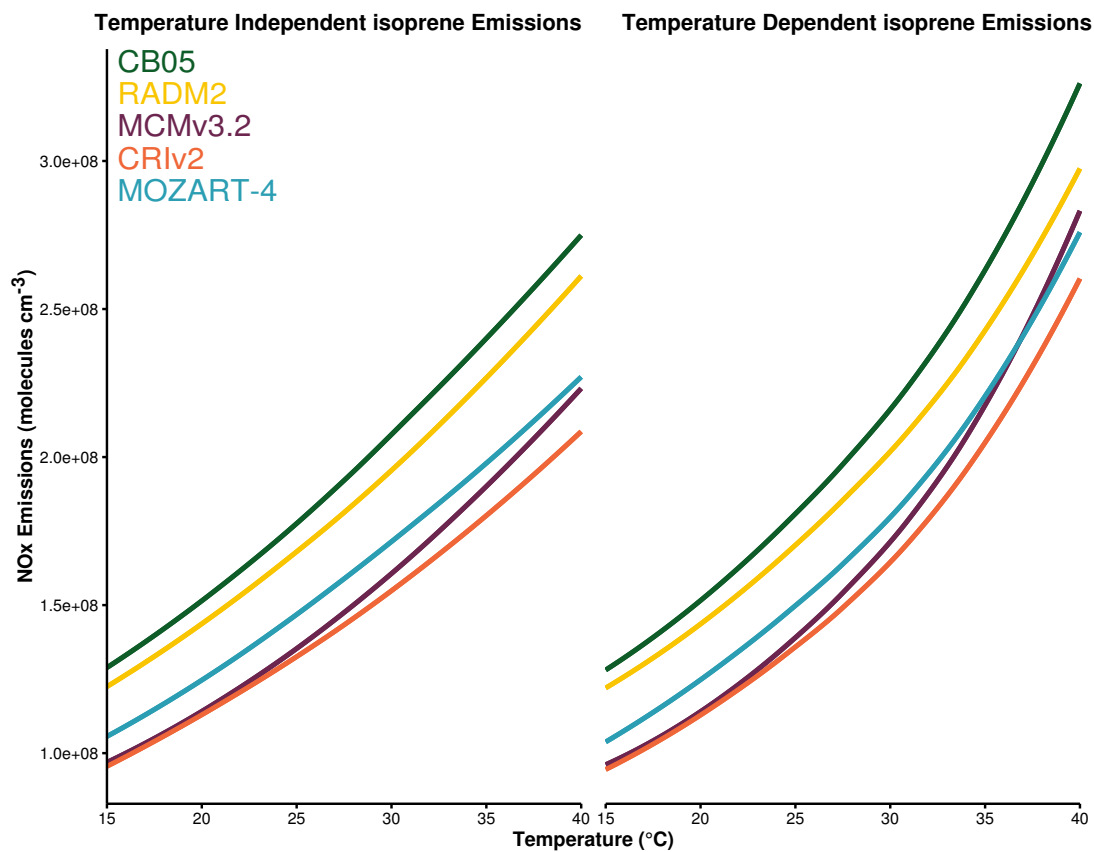
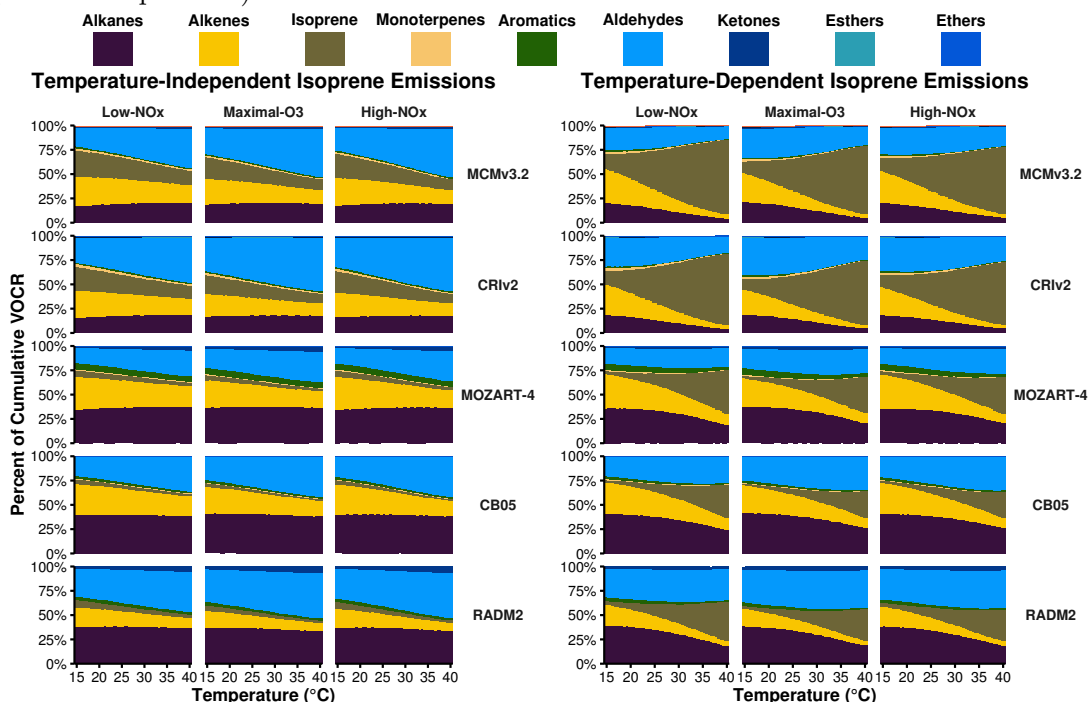


Figure S2: Contributions to cumulative VOC reactivity (VOCR) from different functional groups of emitted VOCs to the total VOCR. Results illustrated at each temperature, for each chemical mechanism and source of isoprene emissions (temperature-independent and temperature-dependent).

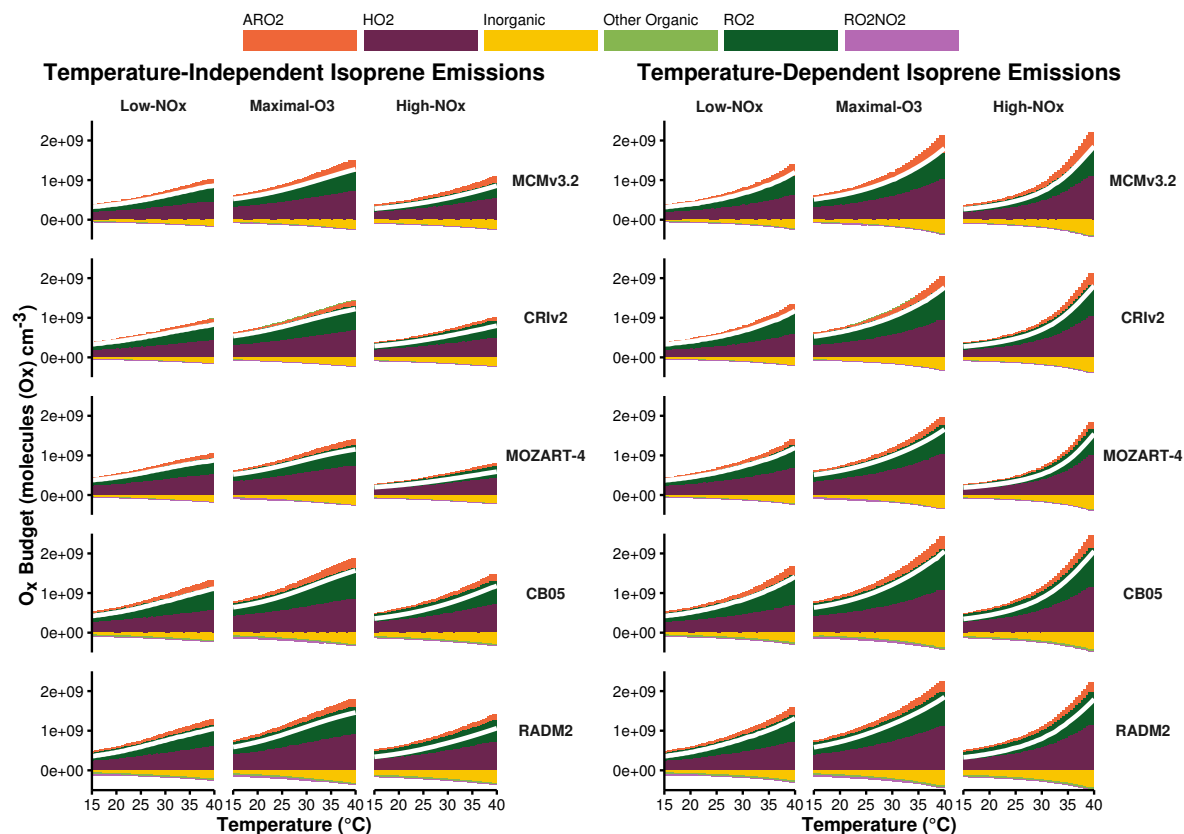


### S3 Ox Production and Consumption Budgets

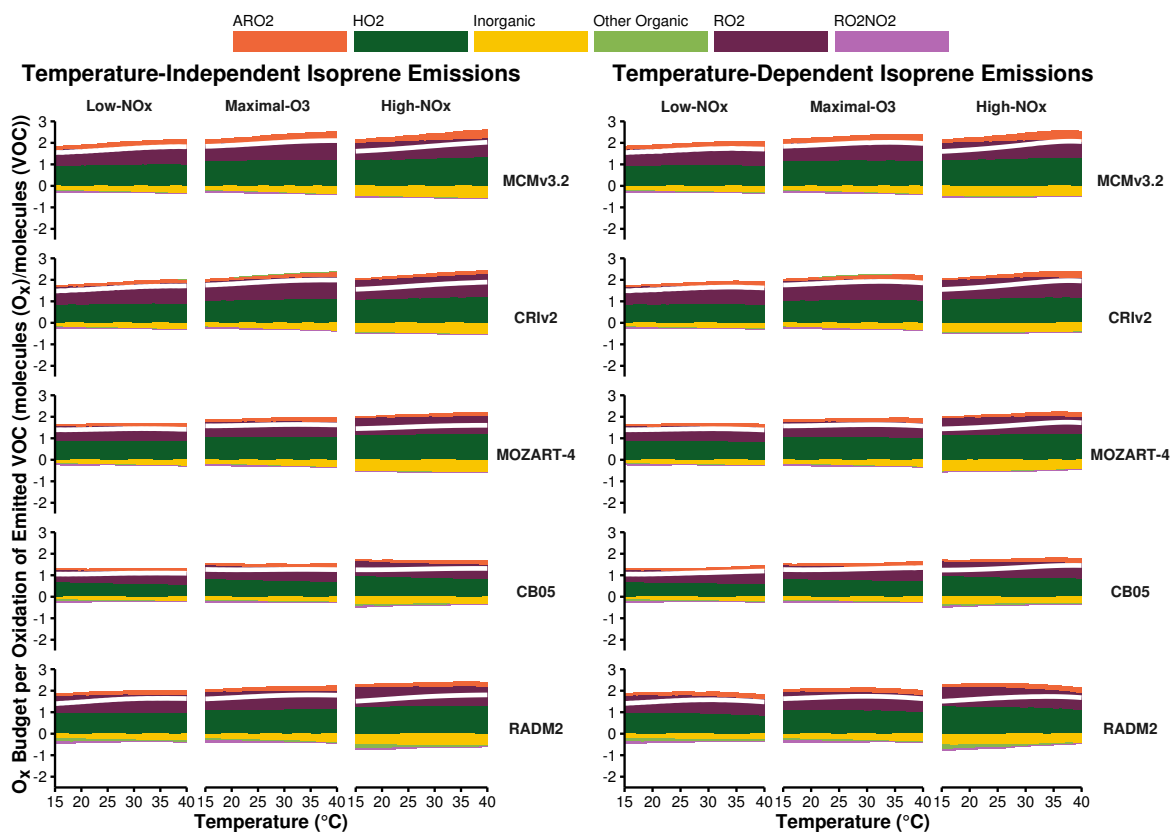
Further box model simulations of stagnant conditions were performed as outlined in Section 3.3 of the research article and an analysis similar to that Section 3.2 of the research article looked at the production and consumption budgets of  $O_x$  was performed. As in Fig. 4 of the research article the 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. 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 loss rate of emitted VOC are displayed in Fig. S3b. These  $O_x$  budgets are displayed for each chemical mechanism,  $NO_x$  condition and source of isoprene emissions (temperature independent and temperature dependent) in Figs. S3a and S3b. This analysis support the conclusion that the 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.



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- 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.