Supplement of Atmos. Chem. Phys., 20, 4905–4931, 2020
https://doi.org/10.5194/acp-20-4905-2020-supplement
© Author(s) 2020. This work is distributed under
the Creative Commons Attribution 4.0 License.

Supplement of

Modeling organic aerosol over Europe in summer conditions with the VBS-GECKO parameterization: sensitivity to secondary organic compound properties and IVOC (intermediate-volatility organic compound) emissions

Victor Lannuque et al.

Correspondence to: Victor Lannuque (victor.lannuque@lisa.u-pec.fr) and Florian Couvidat (florian.couvidat@ineris.fr)

The copyright of individual parts of the supplement might differ from the CC BY 4.0 License.
Table S1 – The H2O mechanism

| Reactions | Kinetic rate parameters (s⁻¹ or molecule⁻¹ cm³ s⁻¹) |
|-----------|-----------------------------------------------|
| ISOP + OH → ISOR + OH | $2.54 \times 10^{-11} \times \exp(408/T)$ |
| ISOP + NO3 → ISON + NO3 | $3.03 \times 10^{-12} \times \exp(448/T)$ |
| ISOR + H2O → 0.28 BiPER + 0.030 BiDER + HO2 | $2.05 \times 10^{-13} \times \exp(1300/T)$ |
| ISOR + C2O3 → 0.026 BiMT + 0.219 MACR + C2O3 | $8.40 \times 10^{-14} \times \exp(221/T)$ |
| ISOR + NO → 0.418 MACR + 0.046 ISON + NO | $3.40 \times 10^{-14} \times \exp(221/T)$ |
| ISOR + NO3 → 0.438 MACR + NO3 | $2.43 \times 10^{-12} \times \exp(360/T)$ |
| ISON + OH → OH | $1.20 \times 10^{-11}$ |
| ISON + NO3 → 0.074 BiNIT3 + NO3 | $6.61 \times 10^{-13}$ |
| MACR + NO → NO | $2.54 \times 10^{-12} \times \exp(360/T)$ |
| MACR + H2O → HO2 | $1.82 \times 10^{-13} \times \exp(1300/T)$ |
| MACR + MeO2 → MeO2 | $3.40 \times 10^{-14} \times \exp(221/T)$ |
| MACR + NO3 → MACR + NO3 | $1.20 \times 10^{-12}$ |
| MPAN + NO → NO | $2.54 \times 10^{-12} \times \exp(360/T)$ |
| MPAN + HO2 → HO2 | $1.82 \times 10^{-13} \times \exp(1300/T)$ |
| MPAN + MeO2 → MeO2 | $3.40 \times 10^{-14} \times \exp(221/T)$ |
| MPAN + NO3 → MPAN + NO3 | $1.60 \times 10^{-14} \times \exp(13486/T)$ |
| BiPER + hν → Degradation products | $k = 50 \times$ kinetic of photolysis of H2O2 |
| API + OH → 0.30 BiA0D + 0.17 BiA1D + 0.10 BiA2D + OH | $1.21 \times 10^{-11} \times \exp(440/T)$ |
| API + O3 → 0.18 BiA0D + 0.26 BiA1D + 0.05 BiA2D + O3 | $5.00 \times 10^{-13} \times \exp(530/T)$ |
| API + NO3 → 0.70 BiA0D + 0.10 BiNIT + NO3 | $1.19 \times 10^{-12} \times \exp(490/T)$ |
| BPI + OH → 0.07 BiA0D + 0.30 BiA1D + 0.06 BiA2D + OH | $3.28 \times 10^{-11} \times \exp(357/T)$ |
| BPI + O3 → 0.09 BiA0D + 0.13 BiA1D + 0.04 BiA2D + O3 | $1.50 \times 10^{-13}$ |
| BPI + NO3 → 0.02 BiA0D + 0.63 BiNIT + NO3 | $2.51 \times 10^{-12}$ |
| LIM + OH → 0.35 BiA0D + 0.20 BiA1D + 0.0035 BiA2D + OH | $4.20 \times 10^{-11} \times \exp(401/T)$ |
| LIM + O3 → 0.09 BiA0D + 0.10 BiA1D + O3 | $2.95 \times 10^{-11} \times \exp(783/T)$ |
| LIM + NO3 → 0.69 BiA0D + 0.27 BiNIT + NO3 | $1.22 \times 10^{-11}$ |
| HUM + OH → 0.74 BiBmP + 0.26 BiBlP + OH | $2.93 \times 10^{-12}$ |
| TOL + OH → ... + 0.25 TOLP | $1.80 \times 10^{-11} \times \exp(355/T)$ |
| TOLP + HO2 → 0.78 AncIP + C2O3 | $1.80 \times 10^{-11} \times \exp(355/T)$ |
| TOLP + C2O3 → 0.78 AncIP + C2O3 | $7.40 \times 10^{-13} \times \exp(765/T)$ |
| TOLP + MeO2 → 0.78 AncIP + MeO2 | $3.56 \times 10^{-14} \times \exp(708/T)$ |
| TOLP + NO → 0.097 AnBmP + 0.748 AnBlP + NO | $2.70 \times 10^{-12} \times \exp(360/T)$ |
| TOLP + NO3 → 0.097 AnBmP + 0.748 AnBlP + NO3 | $1.2 \times 10^{-12}$ |
| XYL + OH → ... + 0.247 XYLP | $1.70 \times 10^{-11} \times \exp(116/T)$ |
| XYLP + HO2 → 0.71 AncIP + HO2 | $3.75 \times 10^{-11} \times \exp(960/T)$ |
| XYLP + C2O3 → 0.71 AncIP + C2O3 | $3.75 \times 10^{-11} \times \exp(960/T)$ |
| XYLP + MeO2 → 0.71 AncIP + MeO2 | $3.56 \times 10^{-14} \times \exp(708/T)$ |
| XYLP + NO → 0.063 AnBmP + 0.424 AnBlP + NO | $2.70 \times 10^{-12} \times \exp(360/T)$ |
| XYLP + NO3 → 0.063 AnBmP + 0.424 AnBlP + NO3 | $1.2 \times 10^{-12}$ |
Table S2 – The VBS-GECKO mechanism as implemented in the ref-VBS-GECKO configuration of CHIMERE (VBs are here named BIO1Bn, BIO2Bn, BIO3Bn, ARO1Bn, ARO2Bn, ARO3Bn, ARO4Bn, ARO5Bn, ALC1Bn, ALC2Bn, and ENE1Bn according to their precursor).

| Reactions | Kinetic rate parameters | Notes |
|-----------|-------------------------|-------|
| **ISOP + OH → ISOR + OH** | $2.54 \times 10^{-11} \exp(408/T)$ | |
| **ISOP + NO3 → ISOR + NO3** | $3.03 \times 10^{-12} \exp(-44/T)$ | |
| **ISOR + HO2 → 0.262 BiPER + 0.030 BiDER + HO2** | $2.05 \times 10^{-13} \exp(1300/T)$ | |
| **ISOR + C2O3 → 0.026 BiMT + 0.219 MACR + C2O3** | $8.40 \times 10^{-14} \exp(221/T)$ | |
| **ISOR + MeO2 → 0.026 BiMT + 0.219 MACR + MeO2** | $3.40 \times 10^{-14} \exp(221/T)$ | |
| **ISOR + NO → 0.418 MACR + 0.046 ISOR + NO** | $2.43 \times 10^{-12} \exp(360/T)$ | |
| **ISOR + NO3 → 0.438 MACR + NO3** | $3.6 \times 10^{-12}$ | |
| **ISOR + OH → OH** | 1.20 $\times 10^{-12}$ | |
| **ISOR + NO3 → 0.074 BiMT3 + NO3** | 1.30 $\times 10^{-11}$ | |
| **MACR + NO → NO** | 6.61 $\times 10^{-13}$ | |
| **MACR + HO2 → HO2** | $1.82 \times 10^{-13} \exp(1300/T)$ | |
| **MACR + MeO2 → MeO2** | $3.0 \times 10^{-14} \exp(221/T)$ | |
| **MACR + NO2 → MPAN + NO2** | $2.80 \times 10^{-12} \exp(181/T)$ | |
| **MPAN → MACR** | $1.60 \times 10^{-10} \exp(-13486/T)$ | |
| **MPAN + OH → 0.067 BiMG4 + 0.047 BiNGA + OH** | 3.20 $\times 10^{-11}$ | |
| **MPAN + NO3 → 0.067 BiMG4 + 0.047 BiNGA + NO3** | 3.20 $\times 10^{-11}$ | |
| **BiPER + hν → Degradation products** | $k = 50 \times$ kinetic of photolysis of H2O2 | |
| **APINEN + OH → a1 BIO1B1 + a2 BIO1B2 + a3 BIO1B3 + a4 BIO1B4 + a5 BIO1B5 + a6 BIO1B6 + a7 BIO1B7 + OH** | $1.21 \times 10^{-11} \exp(440/T)$ | |
| **APINEN + O3 → a1 BIO1B1 + a2 BIO1B2 + a3 BIO1B3 + a4 BIO1B4 + a5 BIO1B5 + a6 BIO1B6 + a7 BIO1B7 + O3** | 5.00 $\times 10^{-16} \exp(-530/T)$ | |
| **APINEN + NO3 → a1 BIO1B1 + a2 BIO1B2 + a3 BIO1B3 + a4 BIO1B4 + a5 BIO1B5 + a6 BIO1B6 + a7 BIO1B7 + NO3** | $1.91 \times 10^{-12} \exp(-490/T)$ | |
| **BIO1B1(1-6) + OH → a1 BIO1B1 + a2 BIO1B2 + a3 BIO1B3 + a4 BIO1B4 + a5 BIO1B5 + a6 BIO1B6 + a7 BIO1B7 + OH** | 4.0 $\times 10^{-11}$ | |
| **BIO1B1(1-6) + hν → Degradation products** | $k = 11.5 \times$ kinetic of photolysis of acetone | |
| **BPINEN + OH → a1 BIO2B1 + a2 BIO2B2 + a3 BIO2B3 + a4 BIO2B4 + a5 BIO2B5 + a6 BIO2B6 + a7 BIO2B7 + OH** | $2.38 \times 10^{-11} \exp(357/T)$ | |
| **BPINEN + O3 → a1 BIO2B1 + a2 BIO2B2 + a3 BIO2B3 + a4 BIO2B4 + a5 BIO2B5 + a6 BIO2B6 + a7 BIO2B7 + O3** | 1.50 $\times 10^{-11}$ | |
| **BPINEN + NO3 → a1 BIO2B1 + a2 BIO2B2 + a3 BIO2B3 + a4 BIO2B4 + a5 BIO2B5 + a6 BIO2B6 + a7 BIO2B7 + NO3** | $2.51 \times 10^{-12}$ | |
| **BIO2B1(1-6) + OH → a1 BIO2B1 + a2 BIO2B2 + a3 BIO2B3 + a4 BIO2B4 + a5 BIO2B5 + a6 BIO2B6 + a7 BIO2B7 + OH** | 4.0 $\times 10^{-11}$ | |
| **BIO2B1(1-6) + hν → Degradation products** | $k = 23.5 \times$ kinetic of photolysis of acetone | |
| **LIMONE + OH → a1 BIO3B1 + a2 BIO3B2 + a3 BIO3B3 + a4 BIO3B4 + a5 BIO3B5 + a6 BIO3B6 + a7 BIO3B7 + OH** | $4.20 \times 10^{-11} \exp(401/T)$ | |
| **LIMONE + O3 → a1 BIO3B1 + a2 BIO3B2 + a3 BIO3B3 + a4 BIO3B4 + a5 BIO3B5 + a6 BIO3B6 + a7 BIO3B7 + O3** | $2.95 \times 10^{-15} \exp(783/T)$ | |
| **LIMONE + NO3 → a1 BIO3B1 + a2 BIO3B2 + a3 BIO3B3 + a4 BIO3B4 + a5 BIO3B5 + a6 BIO3B6 + a7 BIO3B7 + NO3** | $1.22 \times 10^{-11}$ | |
| **BIO3B1(1-6) + OH → a1 BIO3B1 + a2 BIO3B2 + a3 BIO3B3 + a4 BIO3B4 + a5 BIO3B5 + a6 BIO3B6 + a7 BIO3B7 + OH** | 4.0 $\times 10^{-11}$ | |
| **BIO3B1(1-6) + hν → Degradation products** | $k = 23.3 \times$ kinetic of photolysis of acetone | |
| **OCIMEN + OH → a1 BIO3B1 + a2 BIO3B2 + a3 BIO3B3 + a4 BIO3B4 + a5 BIO3B5 + a6 BIO3B6 + a7 BIO3B7 + OH** | 5.10 $\times 10^{-7} / T$ | |
| **OCIMEN + O3 → a1 BIO3B1 + a2 BIO3B2 + a3 BIO3B3 + a4 BIO3B4 + a5 BIO3B5 + a6 BIO3B6 + a7 BIO3B7 + O3** | 7.50 $\times 10^{-8} / T$ | |
| **OCIMEN + NO3 → a1 BIO3B1 + a2 BIO3B2 + a3 BIO3B3 + a4 BIO3B4 + a5 BIO3B5 + a6 BIO3B6 + a7 BIO3B7 + NO3** | 4.30 $\times 10^{-7} / T$ | |
| **HUM + OH → 0.74 BipB2 + 0.26 BipB + OH** | $2.93 \times 10^{-10}$ | |
| **BENZEN + OH → a1 ARO1B1 + a2 ARO1B2 + a3 ARO1B3 + a4 ARO1B4 + a5 ARO1B5 + a6 ARO1B6 + a7 ARO1B7 + OH** | $1.21 \times 10^{-11}$ | |
| **ARO1B1(1-6) + OH → a1 ARO1B1 + a2 ARO1B2 + a3 ARO1B3 + a4 ARO1B4 + a5 ARO1B5 + a6 ARO1B6 + a7 ARO1B7 + OH** | 4.0 $\times 10^{-11}$ | |
| **ARO1B1(1-6) + hν → Degradation products** | $k = 1.50 \times$ kinetic of photolysis of acetone | |
| **TOLUEN + OH → a1 ARO2B1 + a2 ARO2B2 + a3 ARO2B3 + a4 ARO2B4 + a5 ARO2B5 + a6 ARO2B6 + a7 ARO2B7 + OH** | $5.63 \times 10^{-15}$ | |
| **ARO2B1(1-6) + OH → a1 ARO2B1 + a2 ARO2B2 + a3 ARO2B3 + a4 ARO2B4 + a5 ARO2B5 + a6 ARO2B6 + a7 ARO2B7 + OH** | 4.0 $\times 10^{-11}$ | |
| **ARO2B1(1-6) + hν → Degradation products** | $k = 19.9 \times$ kinetic of photolysis of acetone | |
| Reaction | Stoichiometry | Rate Constant | Remarks |
|----------|---------------|---------------|---------|
| OXYLEN + OH → a₁ ARO3B₁ + a₂ ARO3B₂ + a₃ ARO3B₃ + a₄ ARO3B₄ + a₅ ARO3B₅ + a₆ ARO3B₆ + a₇ ARO3B₇ + OH | 1.360 × 10⁻¹¹ | * | *
| OXYLEN + OH → a₁ ARO3B₁ + a₂ ARO3B₂ + a₃ ARO3B₃ + a₄ ARO3B₄ + a₅ ARO3B₅ + a₆ ARO3B₆ + a₇ ARO3B₇ + OH | 4.0 × 10⁻¹¹ | * | *
| MXYLEN + OH → a₁ ARO4B₁ + a₂ ARO4B₂ + a₃ ARO4B₃ + a₄ ARO4B₄ + a₅ ARO4B₅ + a₆ ARO4B₆ + a₇ ARO4B₇ + OH | 2.305 × 10⁻¹⁰ | * | *
| MXYLEN + OH → a₁ ARO4B₁ + a₂ ARO4B₂ + a₃ ARO4B₃ + a₄ ARO4B₄ + a₅ ARO4B₅ + a₆ ARO4B₆ + a₇ ARO4B₇ + OH | 4.0 × 10⁻¹¹ | * | *
| PXYLEN + OH → a₁ ARO5B₁ + a₂ ARO5B₂ + a₃ ARO5B₃ + a₄ ARO5B₄ + a₅ ARO5B₅ + a₆ ARO5B₆ + a₇ ARO5B₇ + OH | 1.431 × 10⁻¹¹ | * | *
| PXYLEN + OH → a₁ ARO5B₁ + a₂ ARO5B₂ + a₃ ARO5B₃ + a₄ ARO5B₄ + a₅ ARO5B₅ + a₆ ARO5B₆ + a₇ ARO5B₇ + OH | 4.0 × 10⁻¹¹ | * | *
| ALC₁₀ + OH → a₁ ALC₁B₁ + a₂ ALC₁B₂ + a₃ ALC₁B₃ + a₄ ALC₁B₄ + a₅ ALC₁B₅ + a₆ ALC₁B₆ + a₇ ALC₁B₇ + OH | 1.099 × 10⁻¹⁰ | * | *
| ALC₁₀ + OH → a₁ ALC₁B₁ + a₂ ALC₁B₂ + a₃ ALC₁B₃ + a₄ ALC₁B₄ + a₅ ALC₁B₅ + a₆ ALC₁B₆ + a₇ ALC₁B₇ + OH | 4.0 × 10⁻¹¹ | * | *
| ALC₁₂B₁ + OH → a₁ ALC₂B₁ + a₂ ALC₂B₂ + a₃ ALC₂B₃ + a₄ ALC₂B₄ + a₅ ALC₂B₅ + a₆ ALC₂B₆ + a₇ ALC₂B₇ + OH | 1.678 × 10⁻¹⁰ | * | *
| ALC₁₂B₁ + OH → a₁ ALC₂B₁ + a₂ ALC₂B₂ + a₃ ALC₂B₃ + a₄ ALC₂B₄ + a₅ ALC₂B₅ + a₆ ALC₂B₆ + a₇ ALC₂B₇ + OH | 4.0 × 10⁻¹¹ | * | *
| ENE₁₀ + OH → a₁ ENE₁B₁ + a₂ ENE₁B₂ + a₃ ENE₁B₃ + a₄ ENE₁B₄ + a₅ ENE₁B₅ + a₆ ENE₁B₆ + a₇ ENE₁B₇ + OH | 4.402 × 10⁻¹¹ | * | *
| ENE₁₀ + OH → a₁ ENE₁B₁ + a₂ ENE₁B₂ + a₃ ENE₁B₃ + a₄ ENE₁B₄ + a₅ ENE₁B₅ + a₆ ENE₁B₆ + a₇ ENE₁B₇ + OH | 9.290 × 10⁻¹⁰ | * | *
| ENE₁₀ + NO₃ → a₁ ENE₁B₁ + a₂ ENE₁B₂ + a₃ ENE₁B₃ + a₄ ENE₁B₄ + a₅ ENE₁B₅ + a₆ ENE₁B₆ + a₇ ENE₁B₇ + NO₃ | 0.265 × 10⁻¹⁰ | * | *
| ENE₁₀ + NO₃ → a₁ ENE₁B₁ + a₂ ENE₁B₂ + a₃ ENE₁B₃ + a₄ ENE₁B₄ + a₅ ENE₁B₅ + a₆ ENE₁B₆ + a₇ ENE₁B₇ + OH | 4.0 × 10⁻¹⁰ | * | *

Reactions in italic are taken from the H₂O mechanism

* the VBₖ are formed according to RRR and reactive species dependent aₖ stoichiometric coefficients (cf Lannuque et al., 2018)
| Reactions | Kinetic rate parameters | Notes |
|-----------|-------------------------|-------|
| ALC14 + OH → a1 ALC2B1 + a2 ALC2B2 + a3 ALC2B3 + a4 ALC2B4 + a5 ALC2B5 + a6 ALC2B6 + a7 ALC2B7 + OH | 1.678 × 10^{-11} | * |
| ALC2B1(1-6) + OH → a1 ALC2B1 + a2 ALC2B2 + a3 ALC2B3 + a4 ALC2B4 + a5 ALC2B5 + a6 ALC2B6 + a7 ALC2B7 + OH | 4.0 × 10^{-11} | * |
| ALC2B1(1-6) + hv → Degradation products | k = 19.4 × kinetic of photolysis of aceton | |
| ALC18 + OH → a1 ALC3B1 + a2 ALC3B2 + a3 ALC3B3 + a4 ALC3B4 + a5 ALC3B5 + a6 ALC3B6 + a7 ALC3B7 + OH | 2.244 × 10^{-11} | * |
| ALC3B1(1-6) + OH → a1 ALC3B1 + a2 ALC3B2 + a3 ALC3B3 + a4 ALC3B4 + a5 ALC3B5 + a6 ALC3B6 + a7 ALC3B7 + OH | 4.0 × 10^{-11} | * |
| ALC3B1(1-6) + hv → Degradation products | k = 6.39 × kinetic of photolysis of aceton | |
| ALC22 + OH → a1 ALC4B1 + a2 ALC4B2 + a3 ALC4B3 + a4 ALC4B4 + a5 ALC4B5 + a6 ALC4B6 + a7 ALC4B7 + OH | 2.811 × 10^{-11} | * |
| ALC4B1(1-6) + OH → a1 ALC4B1 + a2 ALC4B2 + a3 ALC4B3 + a4 ALC4B4 + a5 ALC4B5 + a6 ALC4B6 + a7 ALC4B7 + OH | 4.0 × 10^{-11} | * |
| ALC4B1(1-6) + hv → Degradation products | k = 6.25 × kinetic of photolysis of aceton | |
| ALC26 + OH → a1 ALC5B1 + a2 ALC5B2 + a3 ALC5B3 + a4 ALC5B4 + a5 ALC5B5 + a6 ALC5B6 + a7 ALC5B7 + OH | 3.377 × 10^{-11} | * |
| ALC5B1(1-6) + OH → a1 ALC5B1 + a2 ALC5B2 + a3 ALC5B3 + a4 ALC5B4 + a5 ALC5B5 + a6 ALC5B6 + a7 ALC5B7 + OH | 4.0 × 10^{-11} | * |
| ALC5B1(1-6) + hv → Degradation products | k = 0.00 × kinetic of photolysis of aceton | |
| ENE18 + OH → a1 ENE3B1 + a2 ENE3B2 + a3 ENE3B3 + a4 ENE3B4 + a5 ENE3B5 + a6 ENE3B6 + a7 ENE3B7 + OH | 5.537 × 10^{-11} | * |
| ENE18 + O3 → a1 ENE3B1 + a2 ENE3B2 + a3 ENE3B3 + a4 ENE3B4 + a5 ENE3B5 + a6 ENE3B6 + a7 ENE3B7 + O3 | 1.011 × 10^{-17} | * |
| ENE18 + NO3 → a1 ENE3B1 + a2 ENE3B2 + a3 ENE3B3 + a4 ENE3B4 + a5 ENE3B5 + a6 ENE3B6 + a7 ENE3B7 + NO3 | 0.326 × 10^{-13} | * |
| ENE3B1(1-6) + OH → a1 ENE3B1 + a2 ENE3B2 + a3 ENE3B3 + a4 ENE3B4 + a5 ENE3B5 + a6 ENE3B6 + a7 ENE3B7 + OH | 4.0 × 10^{-11} | * |
| ENE3B1(1-6) + hv → Degradation products | k = 2.74 × kinetic of photolysis of aceton | |
| ENE22 + OH → a1 ENE4B1 + a2 ENE4B2 + a3 ENE4B3 + a4 ENE4B4 + a5 ENE4B5 + a6 ENE4B6 + a7 ENE4B7 + OH | 6.105 × 10^{-11} | * |
| ENE22 + O3 → a1 ENE4B1 + a2 ENE4B2 + a3 ENE4B3 + a4 ENE4B4 + a5 ENE4B5 + a6 ENE4B6 + a7 ENE4B7 + O3 | 1.011 × 10^{-17} | * |
| ENE22 + NO3 → a1 ENE4B1 + a2 ENE4B2 + a3 ENE4B3 + a4 ENE4B4 + a5 ENE4B5 + a6 ENE4B6 + a7 ENE4B7 + NO3 | 0.337 × 10^{-13} | * |
| ENE4B1(1-6) + OH → a1 ENE4B1 + a2 ENE4B2 + a3 ENE4B3 + a4 ENE4B4 + a5 ENE4B5 + a6 ENE4B6 + a7 ENE4B7 + OH | 4.0 × 10^{-11} | * |
| ENE4B1(1-6) + hv → Degradation products | k = 6.13 × kinetic of photolysis of aceton | |
| ENE26 + OH → a1 ENE5B1 + a2 ENE5B2 + a3 ENE5B3 + a4 ENE5B4 + a5 ENE5B5 + a6 ENE5B6 + a7 ENE5B7 + OH | 6.673 × 10^{-11} | * |
| ENE26 + O3 → a1 ENE5B1 + a2 ENE5B2 + a3 ENE5B3 + a4 ENE5B4 + a5 ENE5B5 + a6 ENE5B6 + a7 ENE5B7 + O3 | 1.011 × 10^{-17} | * |
| ENE26 + NO3 → a1 ENE5B1 + a2 ENE5B2 + a3 ENE5B3 + a4 ENE5B4 + a5 ENE5B5 + a6 ENE5B6 + a7 ENE5B7 + NO3 | 0.343 × 10^{-13} | * |
| ENE5B1(1-6) + OH → a1 ENE5B1 + a2 ENE5B2 + a3 ENE5B3 + a4 ENE5B4 + a5 ENE5B5 + a6 ENE5B6 + a7 ENE5B7 + OH | 4.0 × 10^{-11} | * |
| ENE5B1(1-6) + hv → Degradation products | k = 0.00 × kinetic of photolysis of aceton | |

Reactions in italic are already in the ref-VBS-GECKO configuration of CHIMERE.

* the VBS are formed according to RRR and reactive species dependent a$_i$ stoichiometric coefficients (cf Lannuque et al., 2018)
Figure S1 – Mean simulated $\text{emission}_{\text{toluene}}/\text{emission}_{\text{α-pinene}}$ ratio for July-August 2013 over Europe. Circles represent stations used for time series comparison. White pixels represent limit values of the ratio (typically when at least one of the emission fluxes is null).
Figure S2 – Evolution of simulated OA concentrations and distribution function of volatility bins with the IVOC_{SVOC} model configuration (from the less volatile one VB7, to the more volatile VB1). Panels b, d, f and h present mean daily profiles. Results are shown at two stations influenced by anthropogenic sources in Netherlands (NL0644R, a and b) and in France (FR0020R, c and d) and at two stations influenced by biogenic sources in Norway (NL0002R, e and f) and Slovenia (SI0008R, g and h). “Traffic SVOC” includes C_{14} to C_{26} emitted VBS-GECKO alkanes and alkenes and “others” includes all species from H2O mechanism.
Figure S3 – Mean RRR over Europe during the two-month period for the ref-VBS-GECKO model configuration.