

## Supplementary material for

# Modelling organic aerosol over Europe in summer conditions with the VBS-GECKO parameterization: sensitivity to secondary organic compound properties and IVOC emissions

Victor Lannuque<sup>1,2,3,a</sup>, Florian Couvidat<sup>2</sup>, Marie Camredon<sup>1</sup>, Bernard Aumont<sup>1</sup> and Bertrand Bessagnet<sup>2,b</sup>

<sup>1</sup>LISA, UMR CNRS 7583, IPSL, Université Paris Est Créteil and Université Paris Diderot, 94010 Créteil Cedex, France.

<sup>2</sup>INERIS, National Institute for Industrial Environment and Risks, Parc Technologique ALATA, 60550 Verneuil-en-Halatte, France.

<sup>3</sup>Agence de l'Environnement et de la Maîtrise de l'Energie, 20 avenue du Grésillé - BP 90406, 49004 Angers Cedex 01, France.

<sup>a</sup> Now at : Laboratoire d'Aérodologie, Université de Toulouse, CNRS, UPS, Toulouse, France.

<sup>b</sup> Now at : Hangzhou Futuris Environmental Technology Co. Ltd, Zhejiang Overseas High-Level Talent Innovation Park, No. 998 WenYi Road, 311121, Hangzhou, Zhejiang, China.

*Correspondence to:* Victor Lannuque (victor.lannuque@gmail.com) and Florian Couvidat (florian.couvidat@ineris.fr)

**Table S1 – The H<sup>2</sup>O mechanism**

Reactions	Kinetic rate parameters (s <sup>-1</sup> or molecule <sup>-1</sup> .cm <sup>3</sup> .s <sup>-1</sup> )
ISOP + OH → ISOR + OH	2.54 × 10 <sup>-11</sup> × exp(408/T)
ISOP + NO <sub>3</sub> → ISON + NO <sub>3</sub>	3.03 × 10 <sup>-12</sup> × exp(-448/T)
ISOR + HO <sub>2</sub> → 0.282 BiPER + 0.030 BiDER + HO <sub>2</sub>	2.05 × 10 <sup>-13</sup> × exp(1300/T)
ISOR + C <sub>2</sub> O <sub>3</sub> → 0.026 BiMT + 0.219 MACR + C <sub>2</sub> O <sub>3</sub>	8.40 × 10 <sup>-14</sup> × exp(221/T)
ISOR + MeO <sub>2</sub> → 0.026 BiMT + 0.219 MACR + MeO <sub>2</sub>	3.40 × 10 <sup>-14</sup> × exp(221/T)
ISOR + NO → 0.418 MACR + 0.046 ISON + NO	2.43 × 10 <sup>-12</sup> × exp(360/T)
ISOR + NO <sub>3</sub> → 0.438 MACR + NO <sub>3</sub>	1.20 × 10 <sup>-12</sup>
ISON + OH → OH	1.30 × 10 <sup>-11</sup>
ISON + NO <sub>3</sub> → 0.074 BiNIT <sub>3</sub> + NO <sub>3</sub>	6.61 × 10 <sup>-13</sup>
MACR + NO → NO	2.54 × 10 <sup>-12</sup> × exp(360/T)
MACR + HO <sub>2</sub> → HO <sub>2</sub>	1.82 × 10 <sup>-13</sup> × exp(1300/T)
MACR + MeO <sub>2</sub> → MeO <sub>2</sub>	3.40 × 10 <sup>-14</sup> × exp(221/T)
MACR + NO <sub>2</sub> → MPAN + NO <sub>2</sub>	2.80 × 10 <sup>-12</sup> × exp(181/T)
MPAN → MACR	1.60 × 10 <sup>16</sup> × exp(-13486/T)
MPAN + OH → 0.067 BiMGA + 0.047 BiNGA + OH	3.20 × 10 <sup>-11</sup>
MPAN + NO <sub>3</sub> → 0.067 BiMGA + 0.047 BiNGA + NO <sub>3</sub>	3.20 × 10 <sup>-11</sup>
BiPER + hv → Degradation products	k = 50 × kinetic of photolysis of H <sub>2</sub> O <sub>2</sub>
API + OH → 0.30 BiA0D + 0.17 BiA1D + 0.10 BiA2D + OH	1.21 × 10 <sup>-11</sup> × exp(440/T)
API + O <sub>3</sub> → 0.18 BiA0D + 0.16 BiA1D + 0.05 BiA2D + O <sub>3</sub>	5.00 × 10 <sup>-16</sup> × exp(-530/T)
API + NO <sub>3</sub> → 0.70 BiA0D + 0.10 BiNIT + NO <sub>3</sub>	1.19 × 10 <sup>-12</sup> × exp(-490/T)
BPI + OH → 0.07 BiA0D + 0.08 BiA1D + 0.06 BiA2D + OH	2.38 × 10 <sup>-11</sup> × exp(357/T)
BPI + O <sub>3</sub> → 0.09 BiA0D + 0.13 BiA1D + 0.04 BiA2D + O <sub>3</sub>	1.50 × 10 <sup>-17</sup>
BPI + NO <sub>3</sub> → 0.02 BiA0D + 0.63 BiNIT + NO <sub>3</sub>	2.51 × 10 <sup>-12</sup>
LIM + OH → 0.35 BiA0D + 0.20 BiA1D + 0.0035 BiA2D + OH	4.20 × 10 <sup>-11</sup> × exp(401/T)
LIM + O <sub>3</sub> → 0.09 BiA0D + 0.10 BiA1D + O <sub>3</sub>	2.95 × 10 <sup>-15</sup> × exp(783/T)
LIM + NO <sub>3</sub> → 0.69 BiA0D + 0.27 BiNIT + NO <sub>3</sub>	1.22 × 10 <sup>-11</sup>
HUM + OH → 0.74 BiBmP + 0.26 BiBIP + OH	2.93 × 10 <sup>-10</sup>
TOL + OH → ... + 0.25 TOLP	1.80 × 10 <sup>-12</sup> × exp(355/T)
TOLP + HO <sub>2</sub> → 0.78 AnCIP + HO <sub>2</sub>	3.75 × 10 <sup>-13</sup> × exp(980/T)
TOLP + C <sub>2</sub> O <sub>3</sub> → 0.78 AnCIP + C <sub>2</sub> O <sub>3</sub>	7.40 × 10 <sup>-13</sup> × exp(765/T)
TOLP + MeO <sub>2</sub> → 0.78 AnCIP + MeO <sub>2</sub>	3.56 × 10 <sup>-14</sup> × exp(708/T)
TOLP + NO → 0.097 AnBIP + 0.748 AnBmP + NO	2.70 × 10 <sup>-12</sup> × exp(360/T)
TOLP + NO <sub>3</sub> → 0.097 AnBIP + 0.748 AnBmP + NO <sub>3</sub>	1.2 × 10 <sup>-12</sup>
XYL + OH → ... + 0.274 XYLP	1.70 × 10 <sup>-11</sup> × exp(116/T)
XYLP + HO <sub>2</sub> → 0.71 AnCIP + HO <sub>2</sub>	3.75 × 10 <sup>-13</sup> × exp(980/T)
XYLP + C <sub>2</sub> O <sub>3</sub> → 0.71 AnCIP + C <sub>2</sub> O <sub>3</sub>	7.40 × 10 <sup>-13</sup> × exp(765/T)
XYLP + MeO <sub>2</sub> → 0.71 AnCIP + MeO <sub>2</sub>	3.56 × 10 <sup>-14</sup> × exp(708/T)
XYLP + NO → 0.063 AnBIP + 0.424 AnBmP + NO	2.70 × 10 <sup>-12</sup> × exp(360/T)
XYLP + NO <sub>3</sub> → 0.063 AnBIP + 0.424 AnBmP + NO <sub>3</sub>	1.2 × 10 <sup>-12</sup>
POAIP + OH → SOAIP	2.0 × 10 <sup>-11</sup>
POAmP + OH → SOAmP	2.0 × 10 <sup>-11</sup>
POAhP + OH → SOAhP	2.0 × 10 <sup>-11</sup>
BOAIP + OH → BSOAIP	2.0 × 10 <sup>-11</sup>
BOAmP + OH → BSOAmP	2.0 × 10 <sup>-11</sup>
BOAhP + OH → BSOAhP	2.0 × 10 <sup>-11</sup>

Table S2 – The VBS-GECKO mechanism as implemented in the ref-VBS-GECKO configuration of CHIMERE.

Reactions	Kinetic rate parameters (s <sup>-1</sup> or molecule <sup>-1</sup> .cm <sup>3</sup> .s <sup>-1</sup> )	Notes
<i>ISOP + OH → ISOR + OH</i>	$2.54 \times 10^{-11} \times \exp(408/T)$	
<i>ISOP + NO3 → ISON + NO3</i>	$3.03 \times 10^{-12} \times \exp(-448/T)$	
<i>ISOR + HO2 → 0.282 BiPER + 0.030 BiDER + HO2</i>	$2.05 \times 10^{-13} \times \exp(1300/T)$	
<i>ISOR + C2O3 → 0.026 BiMT + 0.219 MACR + C2O3</i>	$8.40 \times 10^{-14} \times \exp(221/T)$	
<i>ISOR + MeO2 → 0.026 BiMT + 0.219 MACR + MeO2</i>	$3.40 \times 10^{-14} \times \exp(221/T)$	
<i>ISOR + NO → 0.418 MACR + 0.046 ISON + NO</i>	$2.43 \times 10^{-12} \times \exp(360/T)$	
<i>ISOR + NO3 → 0.438 MACR + NO3</i>	$1.20 \times 10^{-12}$	
<i>ISON + OH → OH</i>	$1.30 \times 10^{-11}$	
<i>ISON + NO3 → 0.074 BiNIT3 + NO3</i>	$6.61 \times 10^{-13}$	
<i>MACR + NO → NO</i>	$2.54 \times 10^{-12} \times \exp(360/T)$	
<i>MACR + HO2 → HO2</i>	$1.82 \times 10^{-13} \times \exp(1300/T)$	
<i>MACR + MeO2 → MeO2</i>	$3.40 \times 10^{-14} \times \exp(221/T)$	
<i>MACR + NO2 → MPAN + NO2</i>	$2.80 \times 10^{-12} \times \exp(181/T)$	
<i>MPAN → MACR</i>	$1.60 \times 10^{16} \times \exp(-13486/T)$	
<i>MPAN + OH → 0.067 BiMGA + 0.047 BiNGA + OH</i>	$3.20 \times 10^{-11}$	
<i>MPAN + NO3 → 0.067 BiMGA + 0.047 BiNGA + NO3</i>	$3.20 \times 10^{-11}$	
<i>BiPER + hv → Degradation products</i>	$k = 50 \times \text{kinetic of photolysis of H}_2\text{O}_2$	
<i>APINEN + OH → a<sub>1</sub> BIO1B1 + a<sub>2</sub> BIO1B2 + a<sub>3</sub> BIO1B3 + a<sub>4</sub> BIO1B4 + a<sub>5</sub> BIO1B5 + a<sub>6</sub> BIO1B6 + a<sub>7</sub> BIO1B7 + OH</i>	$1.21 \times 10^{-11} \times \exp(440/T)$	*
<i>APINEN + O3 → a<sub>1</sub> BIO1B1 + a<sub>2</sub> BIO1B2 + a<sub>3</sub> BIO1B3 + a<sub>4</sub> BIO1B4 + a<sub>5</sub> BIO1B5 + a<sub>6</sub> BIO1B6 + a<sub>7</sub> BIO1B7 + O3</i>	$5.00 \times 10^{-16} \times \exp(-530/T)$	*
<i>APINEN + NO3 → a<sub>1</sub> BIO1B1 + a<sub>2</sub> BIO1B2 + a<sub>3</sub> BIO1B3 + a<sub>4</sub> BIO1B4 + a<sub>5</sub> BIO1B5 + a<sub>6</sub> BIO1B6 + a<sub>7</sub> BIO1B7 + NO3</i>	$1.19 \times 10^{-12} \times \exp(-490/T)$	*
<i>BIO1B(1-6) + OH → a<sub>1</sub> BIO1B1 + a<sub>2</sub> BIO1B2 + a<sub>3</sub> BIO1B3 + a<sub>4</sub> BIO1B4 + a<sub>5</sub> BIO1B5 + a<sub>6</sub> BIO1B6 + a<sub>7</sub> BIO1B7 + OH</i>	$4.0 \times 10^{-11}$	*
<i>BIO1B(1-6) + hv → Degradation products</i>	$k = 11.5 \times \text{kinetic of photolysis of acetone}$	
<i>BPINEN + OH → a<sub>1</sub> BIO2B1 + a<sub>2</sub> BIO2B2 + a<sub>3</sub> BIO2B3 + a<sub>4</sub> BIO2B4 + a<sub>5</sub> BIO2B5 + a<sub>6</sub> BIO2B6 + a<sub>7</sub> BIO2B7 + OH</i>	$2.38 \times 10^{-11} \times \exp(357/T)$	*
<i>BPINEN + O3 → a<sub>1</sub> BIO2B1 + a<sub>2</sub> BIO2B2 + a<sub>3</sub> BIO2B3 + a<sub>4</sub> BIO2B4 + a<sub>5</sub> BIO2B5 + a<sub>6</sub> BIO2B6 + a<sub>7</sub> BIO2B7 + O3</i>	$1.50 \times 10^{-17}$	*
<i>BPINEN + NO3 → a<sub>1</sub> BIO2B1 + a<sub>2</sub> BIO2B2 + a<sub>3</sub> BIO2B3 + a<sub>4</sub> BIO2B4 + a<sub>5</sub> BIO2B5 + a<sub>6</sub> BIO2B6 + a<sub>7</sub> BIO2B7 + NO3</i>	$2.51 \times 10^{-12}$	*
<i>BIO2B(1-6) + OH → a<sub>1</sub> BIO2B1 + a<sub>2</sub> BIO2B2 + a<sub>3</sub> BIO2B3 + a<sub>4</sub> BIO2B4 + a<sub>5</sub> BIO2B5 + a<sub>6</sub> BIO2B6 + a<sub>7</sub> BIO2B7 + OH</i>	$4.0 \times 10^{-11}$	*
<i>BIO2B(1-6) + hv → Degradation products</i>	$k = 23.5 \times \text{kinetic of photolysis of acetone}$	
<i>LIMONE + OH → a<sub>1</sub> BIO3B1 + a<sub>2</sub> BIO3B2 + a<sub>3</sub> BIO3B3 + a<sub>4</sub> BIO3B4 + a<sub>5</sub> BIO3B5 + a<sub>6</sub> BIO3B6 + a<sub>7</sub> BIO3B7 + OH</i>	$4.20 \times 10^{-11} \times \exp(401/T)$	*
<i>LIMONE + O3 → a<sub>1</sub> BIO3B1 + a<sub>2</sub> BIO3B2 + a<sub>3</sub> BIO3B3 + a<sub>4</sub> BIO3B4 + a<sub>5</sub> BIO3B5 + a<sub>6</sub> BIO3B6 + a<sub>7</sub> BIO3B7 + O3</i>	$2.95 \times 10^{-15} \times \exp(783/T)$	*
<i>LIMONE + NO3 → a<sub>1</sub> BIO3B1 + a<sub>2</sub> BIO3B2 + a<sub>3</sub> BIO3B3 + a<sub>4</sub> BIO3B4 + a<sub>5</sub> BIO3B5 + a<sub>6</sub> BIO3B6 + a<sub>7</sub> BIO3B7 + NO3</i>	$1.22 \times 10^{-11}$	*
<i>BIO3B(1-6) + OH → a<sub>1</sub> BIO3B1 + a<sub>2</sub> BIO3B2 + a<sub>3</sub> BIO3B3 + a<sub>4</sub> BIO3B4 + a<sub>5</sub> BIO3B5 + a<sub>6</sub> BIO3B6 + a<sub>7</sub> BIO3B7 + OH</i>	$4.0 \times 10^{-11}$	*
<i>BIO3B(1-6) + hv → Degradation products</i>	$k = 23.3 \times \text{kinetic of photolysis of acetone}$	
<i>OCIMEN + OH → a<sub>1</sub> BIO3B1 + a<sub>2</sub> BIO3B2 + a<sub>3</sub> BIO3B3 + a<sub>4</sub> BIO3B4 + a<sub>5</sub> BIO3B5 + a<sub>6</sub> BIO3B6 + a<sub>7</sub> BIO3B7 + OH</i>	$5.10 \times 10^{-8} / T$	*
<i>OCIMEN + O3 → a<sub>1</sub> BIO3B1 + a<sub>2</sub> BIO3B2 + a<sub>3</sub> BIO3B3 + a<sub>4</sub> BIO3B4 + a<sub>5</sub> BIO3B5 + a<sub>6</sub> BIO3B6 + a<sub>7</sub> BIO3B7 + O3</i>	$7.50 \times 10^{-14} / T$	*
<i>OCIMEN + NO3 → a<sub>1</sub> BIO3B1 + a<sub>2</sub> BIO3B2 + a<sub>3</sub> BIO3B3 + a<sub>4</sub> BIO3B4 + a<sub>5</sub> BIO3B5 + a<sub>6</sub> BIO3B6 + a<sub>7</sub> BIO3B7 + NO3</i>	$4.30 \times 10^{-9} / T$	*
<i>HUM + OH → 0.74 BiBmP + 0.26 BiBIP + OH</i>	$2.93 \times 10^{-10}$	
<i>BENZEN + OH → a<sub>1</sub> ARO1B1 + a<sub>2</sub> ARO1B2 + a<sub>3</sub> ARO1B3 + a<sub>4</sub> ARO1B4 + a<sub>5</sub> ARO1B5 + a<sub>6</sub> ARO1B6 + a<sub>7</sub> ARO1B7 + OH</i>	$1.216 \times 10^{-12}$	*
<i>ARO1B(1-6) + OH → a<sub>1</sub> ARO1B1 + a<sub>2</sub> ARO1B2 + a<sub>3</sub> ARO1B3 + a<sub>4</sub> ARO1B4 + a<sub>5</sub> ARO1B5 + a<sub>6</sub> ARO1B6 + a<sub>7</sub> ARO1B7 + OH</i>	$4.0 \times 10^{-11}$	*
<i>ARO1B(1-6) + hv → Degradation products</i>	$k = 1.50 \times \text{kinetic of photolysis of acetone}$	
<i>TOLUEN + OH → a<sub>1</sub> ARO2B1 + a<sub>2</sub> ARO2B2 + a<sub>3</sub> ARO2B3 + a<sub>4</sub> ARO2B4 + a<sub>5</sub> ARO2B5 + a<sub>6</sub> ARO2B6 + a<sub>7</sub> ARO2B7 + OH</i>	$5.639 \times 10^{-12}$	*
<i>ARO2B(1-6) + OH → a<sub>1</sub> ARO2B1 + a<sub>2</sub> ARO2B2 + a<sub>3</sub> ARO2B3 + a<sub>4</sub> ARO2B4 + a<sub>5</sub> ARO2B5 + a<sub>6</sub> ARO2B6 + a<sub>7</sub> ARO2B7 + OH</i>	$4.0 \times 10^{-11}$	*
<i>ARO2B(1-6) + hv → Degradation products</i>	$k = 19.9 \times \text{kinetic of photolysis of acetone}$	
<i>OXYLEN + OH → a<sub>1</sub> ARO3B1 + a<sub>2</sub> ARO3B2 + a<sub>3</sub> ARO3B3 + a<sub>4</sub> ARO3B4 + a<sub>5</sub> ARO3B5 + a<sub>6</sub> ARO3B6 + a<sub>7</sub> ARO3B7 + OH</i>	$1.360 \times 10^{-11}$	*

ARO3B(1-6) + OH → a <sub>1</sub> ARO3B1 + a <sub>2</sub> ARO3B2 + a <sub>3</sub> ARO3B3 + a <sub>4</sub> ARO3B4 + a <sub>5</sub> ARO3B5 + a <sub>6</sub> ARO3B6 + a <sub>7</sub> ARO3B7 + OH	4.0 × 10 <sup>-11</sup>	*
ARO3B(1-6) + hv → Degradation products	k = 2.30 × kinetic of photolysis of acetone	
MXYLEN + OH → a <sub>1</sub> ARO4B1 + a <sub>2</sub> ARO4B2 + a <sub>3</sub> ARO4B3 + a <sub>4</sub> ARO4B4 + a <sub>5</sub> ARO4B5 + a <sub>6</sub> ARO4B6 + a <sub>7</sub> ARO4B7 + OH	2.305 × 10 <sup>-11</sup>	*
ARO4B(1-6) + OH → a <sub>1</sub> ARO4B1 + a <sub>2</sub> ARO4B2 + a <sub>3</sub> ARO4B3 + a <sub>4</sub> ARO4B4 + a <sub>5</sub> ARO4B5 + a <sub>6</sub> ARO4B6 + a <sub>7</sub> ARO4B7 + OH	4.0 × 10 <sup>-11</sup>	*
ARO4B(1-6) + hv → Degradation products	k = 2.59 × kinetic of photolysis of acetone	
PXYLEN + OH → a <sub>1</sub> ARO5B1 + a <sub>2</sub> ARO5B2 + a <sub>3</sub> ARO5B3 + a <sub>4</sub> ARO5B4 + a <sub>5</sub> ARO5B5 + a <sub>6</sub> ARO5B6 + a <sub>7</sub> ARO5B7 + OH	1.431 × 10 <sup>-11</sup>	*
ARO5B(1-6) + OH → a <sub>1</sub> ARO5B1 + a <sub>2</sub> ARO5B2 + a <sub>3</sub> ARO5B3 + a <sub>4</sub> ARO5B4 + a <sub>5</sub> ARO5B5 + a <sub>6</sub> ARO5B6 + a <sub>7</sub> ARO5B7 + OH	4.0 × 10 <sup>-11</sup>	*
ARO5B(1-6) + hv → Degradation products	k = 16.4 × kinetic of photolysis of acetone	
ALC10 + OH → a <sub>1</sub> ALC1B1 + a <sub>2</sub> ALC1B2 + a <sub>3</sub> ALC1B3 + a <sub>4</sub> ALC1B4 + a <sub>5</sub> ALC1B5 + a <sub>6</sub> ALC1B6 + a <sub>7</sub> ALC1B7 + OH	1.099 × 10 <sup>-11</sup>	*
ALC1B(1-6) + OH → a <sub>1</sub> ALC1B1 + a <sub>2</sub> ALC1B2 + a <sub>3</sub> ALC1B3 + a <sub>4</sub> ALC1B4 + a <sub>5</sub> ALC1B5 + a <sub>6</sub> ALC1B6 + a <sub>7</sub> ALC1B7 + OH	4.0 × 10 <sup>-11</sup>	*
ALC1B(1-6) + hv → Degradation products	k = 19.1 × kinetic of photolysis of acetone	
ALC14 + OH → a <sub>1</sub> ALC2B1 + a <sub>2</sub> ALC2B2 + a <sub>3</sub> ALC2B3 + a <sub>4</sub> ALC2B4 + a <sub>5</sub> ALC2B5 + a <sub>6</sub> ALC2B6 + a <sub>7</sub> ALC2B7 + OH	1.678 × 10 <sup>-11</sup>	*
ALC2B(1-6) + OH → a <sub>1</sub> ALC2B1 + a <sub>2</sub> ALC2B2 + a <sub>3</sub> ALC2B3 + a <sub>4</sub> ALC2B4 + a <sub>5</sub> ALC2B5 + a <sub>6</sub> ALC2B6 + a <sub>7</sub> ALC2B7 + OH	4.0 × 10 <sup>-11</sup>	*
ALC2B(1-6) + hv → Degradation products	k = 19.4 × kinetic of photolysis of acetone	
ENE10 + OH → a <sub>1</sub> ENE1B1 + a <sub>2</sub> ENE1B2 + a <sub>3</sub> ENE1B3 + a <sub>4</sub> ENE1B4 + a <sub>5</sub> ENE1B5 + a <sub>6</sub> ENE1B6 + a <sub>7</sub> ENE1B7 + OH	4.402 × 10 <sup>-11</sup>	*
ENE10 + O3 → a <sub>1</sub> ENE1B1 + a <sub>2</sub> ENE1B2 + a <sub>3</sub> ENE1B3 + a <sub>4</sub> ENE1B4 + a <sub>5</sub> ENE1B5 + a <sub>6</sub> ENE1B6 + a <sub>7</sub> ENE1B7 + O3	9.290 × 10 <sup>-18</sup>	*
ENE10 + NO3 → a <sub>1</sub> ENE1B1 + a <sub>2</sub> ENE1B2 + a <sub>3</sub> ENE1B3 + a <sub>4</sub> ENE1B4 + a <sub>5</sub> ENE1B5 + a <sub>6</sub> ENE1B6 + a <sub>7</sub> ENE1B7 + NO3	0.265 × 10 <sup>-13</sup>	*
ENE1B(1-6) + OH → a <sub>1</sub> ENE1B1 + a <sub>2</sub> ENE1B2 + a <sub>3</sub> ENE1B3 + a <sub>4</sub> ENE1B4 + a <sub>5</sub> ENE1B5 + a <sub>6</sub> ENE1B6 + a <sub>7</sub> ENE1B7 + OH	4.0 × 10 <sup>-11</sup>	*
ENE1B(1-6) + hv → Degradation products	k = 17.6 × kinetic of photolysis of acetone	
<i>POAIP + OH → SOAIP</i>	2.0 × 10 <sup>-11</sup>	
<i>POAmP + OH → SOAmP</i>	2.0 × 10 <sup>-11</sup>	
<i>POAhP + OH → SOAhP</i>	2.0 × 10 <sup>-11</sup>	
<i>BOAIP + OH → BSOAIP</i>	2.0 × 10 <sup>-11</sup>	
<i>BOAmP + OH → BSOAmP</i>	2.0 × 10 <sup>-11</sup>	
<i>BOAhP + OH → BSOAhP</i>	2.0 × 10 <sup>-11</sup>	

Reactions in italic are taken from the H<sub>2</sub>O mechanism

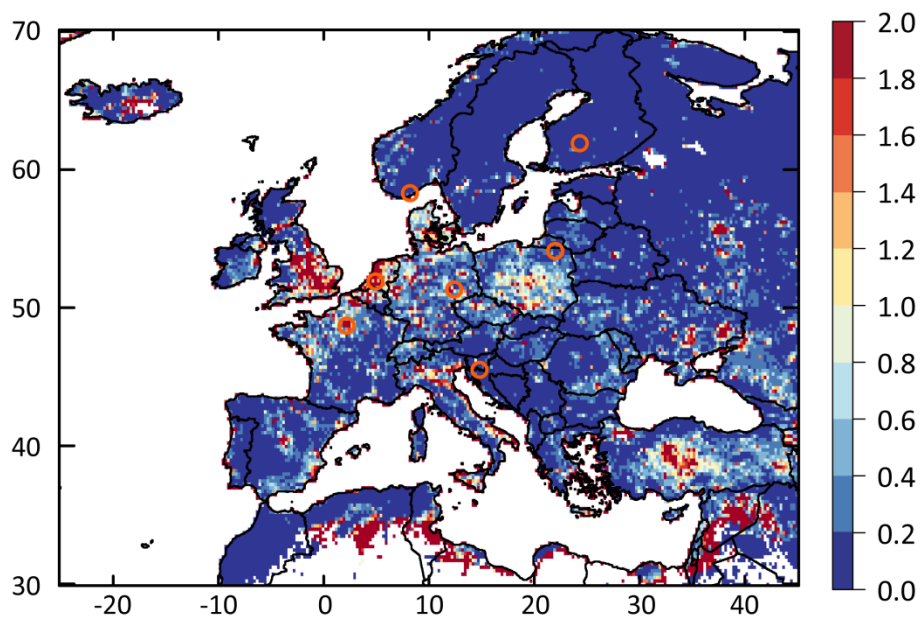
\* the VB(1-7) are formed according to RRR and reactive species dependent a<sub>x</sub> stoichiometric coefficients (cf Lannuque et al., 2018)

Table S3 – The VBS-GECKO mechanism for IVOC and SVOC as implemented in CHIMERE.

Reactions	Kinetic rate parameters (s <sup>-1</sup> or molecule <sup>-1</sup> .cm <sup>3</sup> .s <sup>-1</sup> )	Notes
<i>ALC14 + OH → a<sub>1</sub> ALC2B1 + a<sub>2</sub> ALC2B2 + a<sub>3</sub> ALC2B3 + a<sub>4</sub> ALC2B4 + a<sub>5</sub> ALC2B5 + a<sub>6</sub> ALC2B6 + a<sub>7</sub> ALC2B7 + OH</i>	1.678 × 10 <sup>-11</sup>	*
<i>ALC2B(1-6) + OH → a<sub>1</sub> ALC2B1 + a<sub>2</sub> ALC2B2 + a<sub>3</sub> ALC2B3 + a<sub>4</sub> ALC2B4 + a<sub>5</sub> ALC2B5 + a<sub>6</sub> ALC2B6 + a<sub>7</sub> ALC2B7 + OH</i>	4.0 × 10 <sup>-11</sup>	*
<i>ALC2B(1-6) + hv → Degradation products</i>	k = 19.4 × kinetic of photolysis of acetone	
<i>ALC18 + OH → a<sub>1</sub> ALC3B1 + a<sub>2</sub> ALC3B2 + a<sub>3</sub> ALC3B3 + a<sub>4</sub> ALC3B4 + a<sub>5</sub> ALC3B5 + a<sub>6</sub> ALC3B6 + a<sub>7</sub> ALC3B7 + OH</i>	2.244 × 10 <sup>-11</sup>	*
<i>ALC3Bq(1-6) + OH → a<sub>1</sub> ALC3B1 + a<sub>2</sub> ALC3B2 + a<sub>3</sub> ALC3B3 + a<sub>4</sub> ALC3B4 + a<sub>5</sub> ALC3B5 + a<sub>6</sub> ALC3B6 + a<sub>7</sub> ALC3B7 + OH</i>	4.0 × 10 <sup>-11</sup>	*
<i>ALC3B(1-6) + hv → Degradation products</i>	k = 6.39 × kinetic of photolysis of acetone	
<i>ALC22 + OH → a<sub>1</sub> ALC4B1 + a<sub>2</sub> ALC4B2 + a<sub>3</sub> ALC4B3 + a<sub>4</sub> ALC4B4 + a<sub>5</sub> ALC4B5 + a<sub>6</sub> ALC4B6 + a<sub>7</sub> ALC4B7 + OH</i>	2.811 × 10 <sup>-11</sup>	*
<i>ALC4B(1-6) + OH → a<sub>1</sub> ALC4B1 + a<sub>2</sub> ALC4B2 + a<sub>3</sub> ALC4B3 + a<sub>4</sub> ALC4B4 + a<sub>5</sub> ALC4B5 + a<sub>6</sub> ALC4B6 + a<sub>7</sub> ALC4B7 + OH</i>	4.0 × 10 <sup>-11</sup>	*
<i>ALC4B(1-6) + hv → Degradation products</i>	k = 6.25 × kinetic of photolysis of acetone	
<i>ALC26 + OH → a<sub>1</sub> ALC5B1 + a<sub>2</sub> ALC5B2 + a<sub>3</sub> ALC5B3 + a<sub>4</sub> ALC5B4 + a<sub>5</sub> ALC5B5 + a<sub>6</sub> ALC5B6 + a<sub>7</sub> ALC5B7 + OH</i>	3.377 × 10 <sup>-11</sup>	*
<i>ALC5B(1-6) + OH → a<sub>1</sub> ALC5B1 + a<sub>2</sub> ALC5B2 + a<sub>3</sub> ALC5B3 + a<sub>4</sub> ALC5B4 + a<sub>5</sub> ALC5B5 + a<sub>6</sub> ALC5B6 + a<sub>7</sub> ALC5B7 + OH</i>	4.0 × 10 <sup>-11</sup>	*
<i>ALC5B(1-6) + hv → Degradation products</i>	k = 0.00 × kinetic of photolysis of acetone	
<i>ENE14 + OH → a<sub>1</sub> ENE2B1 + a<sub>2</sub> ENE2B2 + a<sub>3</sub> ENE2B3 + a<sub>4</sub> ENE2B4 + a<sub>5</sub> ENE2B5 + a<sub>6</sub> ENE2B6 + a<sub>7</sub> ENE2B7 + OH</i>	4.970 × 10 <sup>-11</sup>	*
<i>ENE14 + O3 → a<sub>1</sub> ENE2B1 + a<sub>2</sub> ENE2B2 + a<sub>3</sub> ENE2B3 + a<sub>4</sub> ENE2B4 + a<sub>5</sub> ENE2B5 + a<sub>6</sub> ENE2B6 + a<sub>7</sub> ENE2B7 + O3</i>	1.011 × 10 <sup>-17</sup>	*
<i>ENE14 + NO3 → a<sub>1</sub> ENE2B1 + a<sub>2</sub> ENE2B2 + a<sub>3</sub> ENE2B3 + a<sub>4</sub> ENE2B4 + a<sub>5</sub> ENE2B5 + a<sub>6</sub> ENE2B6 + a<sub>7</sub> ENE2B7 + NO3</i>	0.305 × 10 <sup>-13</sup>	*
<i>ENE2B(1-6) + OH → a<sub>1</sub> ENE2B1 + a<sub>2</sub> ENE2B2 + a<sub>3</sub> ENE2B3 + a<sub>4</sub> ENE2B4 + a<sub>5</sub> ENE2B5 + a<sub>6</sub> ENE2B6 + a<sub>7</sub> ENE2B7 + OH</i>	4.0 × 10 <sup>-11</sup>	*
<i>ENE2B(1-6) + hv → Degradation products</i>	k = 9.26 × kinetic of photolysis of acetone	
<i>ENE18 + OH → a<sub>1</sub> ENE3B1 + a<sub>2</sub> ENE3B2 + a<sub>3</sub> ENE3B3 + a<sub>4</sub> ENE3B4 + a<sub>5</sub> ENE3B5 + a<sub>6</sub> ENE3B6 + a<sub>7</sub> ENE3B7 + OH</i>	5.537 × 10 <sup>-11</sup>	*
<i>ENE18 + O3 → a<sub>1</sub> ENE3B1 + a<sub>2</sub> ENE3B2 + a<sub>3</sub> ENE3B3 + a<sub>4</sub> ENE3B4 + a<sub>5</sub> ENE3B5 + a<sub>6</sub> ENE3B6 + a<sub>7</sub> ENE3B7 + O3</i>	1.011 × 10 <sup>-17</sup>	*
<i>ENE18 + NO3 → a<sub>1</sub> ENE3B1 + a<sub>2</sub> ENE3B2 + a<sub>3</sub> ENE3B3 + a<sub>4</sub> ENE3B4 + a<sub>5</sub> ENE3B5 + a<sub>6</sub> ENE3B6 + a<sub>7</sub> ENE3B7 + NO3</i>	0.326 × 10 <sup>-13</sup>	*
<i>ENE3B(1-6) + OH → a<sub>1</sub> ENE3B1 + a<sub>2</sub> ENE3B2 + a<sub>3</sub> ENE3B3 + a<sub>4</sub> ENE3B4 + a<sub>5</sub> ENE3B5 + a<sub>6</sub> ENE3B6 + a<sub>7</sub> ENE3B7 + OH</i>	4.0 × 10 <sup>-11</sup>	*
<i>ENE3B(1-6) + hv → Degradation products</i>	k = 2.74 × kinetic of photolysis of acetone	
<i>ENE22 + OH → a<sub>1</sub> ENE4B1 + a<sub>2</sub> ENE4B2 + a<sub>3</sub> ENE4B3 + a<sub>4</sub> ENE4B4 + a<sub>5</sub> ENE4B5 + a<sub>6</sub> ENE4B6 + a<sub>7</sub> ENE4B7 + OH</i>	6.105 × 10 <sup>-11</sup>	*
<i>ENE22 + O3 → a<sub>1</sub> ENE4B1 + a<sub>2</sub> ENE4B2 + a<sub>3</sub> ENE4B3 + a<sub>4</sub> ENE4B4 + a<sub>5</sub> ENE4B5 + a<sub>6</sub> ENE4B6 + a<sub>7</sub> ENE4B7 + O3</i>	1.011 × 10 <sup>-17</sup>	*
<i>ENE22 + NO3 → a<sub>1</sub> ENE4B1 + a<sub>2</sub> ENE4B2 + a<sub>3</sub> ENE4B3 + a<sub>4</sub> ENE4B4 + a<sub>5</sub> ENE4B5 + a<sub>6</sub> ENE4B6 + a<sub>7</sub> ENE4B7 + NO3</i>	0.337 × 10 <sup>-13</sup>	*
<i>ENE4B(1-6) + OH → a<sub>1</sub> ENE4B1 + a<sub>2</sub> ENE4B2 + a<sub>3</sub> ENE4B3 + a<sub>4</sub> ENE4B4 + a<sub>5</sub> ENE4B5 + a<sub>6</sub> ENE4B6 + a<sub>7</sub> ENE4B7 + OH</i>	4.0 × 10 <sup>-11</sup>	*
<i>ENE4B(1-6) + hv → Degradation products</i>	k = 6.13 × kinetic of photolysis of acetone	
<i>ENE26 + OH → a<sub>1</sub> ENE5B1 + a<sub>2</sub> ENE5B2 + a<sub>3</sub> ENE5B3 + a<sub>4</sub> ENE5B4 + a<sub>5</sub> ENE5B5 + a<sub>6</sub> ENE5B6 + a<sub>7</sub> ENE5B7 + OH</i>	6.673 × 10 <sup>-11</sup>	*
<i>ENE26 + O3 → a<sub>1</sub> ENE5B1 + a<sub>2</sub> ENE5B2 + a<sub>3</sub> ENE5B3 + a<sub>4</sub> ENE5B4 + a<sub>5</sub> ENE5B5 + a<sub>6</sub> ENE5B6 + a<sub>7</sub> ENE5B7 + O3</i>	1.011 × 10 <sup>-17</sup>	*
<i>ENE26 + NO3 → a<sub>1</sub> ENE5B1 + a<sub>2</sub> ENE5B2 + a<sub>3</sub> ENE5B3 + a<sub>4</sub> ENE5B4 + a<sub>5</sub> ENE5B5 + a<sub>6</sub> ENE5B6 + a<sub>7</sub> ENE5B7 + NO3</i>	0.343 × 10 <sup>-13</sup>	*
<i>ENE5B(1-6) + OH → a<sub>1</sub> ENE5B1 + a<sub>2</sub> ENE5B2 + a<sub>3</sub> ENE5B3 + a<sub>4</sub> ENE5B4 + a<sub>5</sub> ENE5B5 + a<sub>6</sub> ENE5B6 + a<sub>7</sub> ENE5B7 + OH</i>	4.0 × 10 <sup>-11</sup>	*
<i>ENE5B(1-6) + hv → Degradation products</i>	k = 0.00 × kinetic of photolysis of acetone	

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

\* the VB(1-7) are formed according to RRR and reactive species dependent a<sub>x</sub> stoichiometric coefficients (cf Lannuque et al., 2018)



5 **Figure S1 – Mean simulated emission<sub>toluene</sub>/emission<sub>α-pinene</sub> 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).**

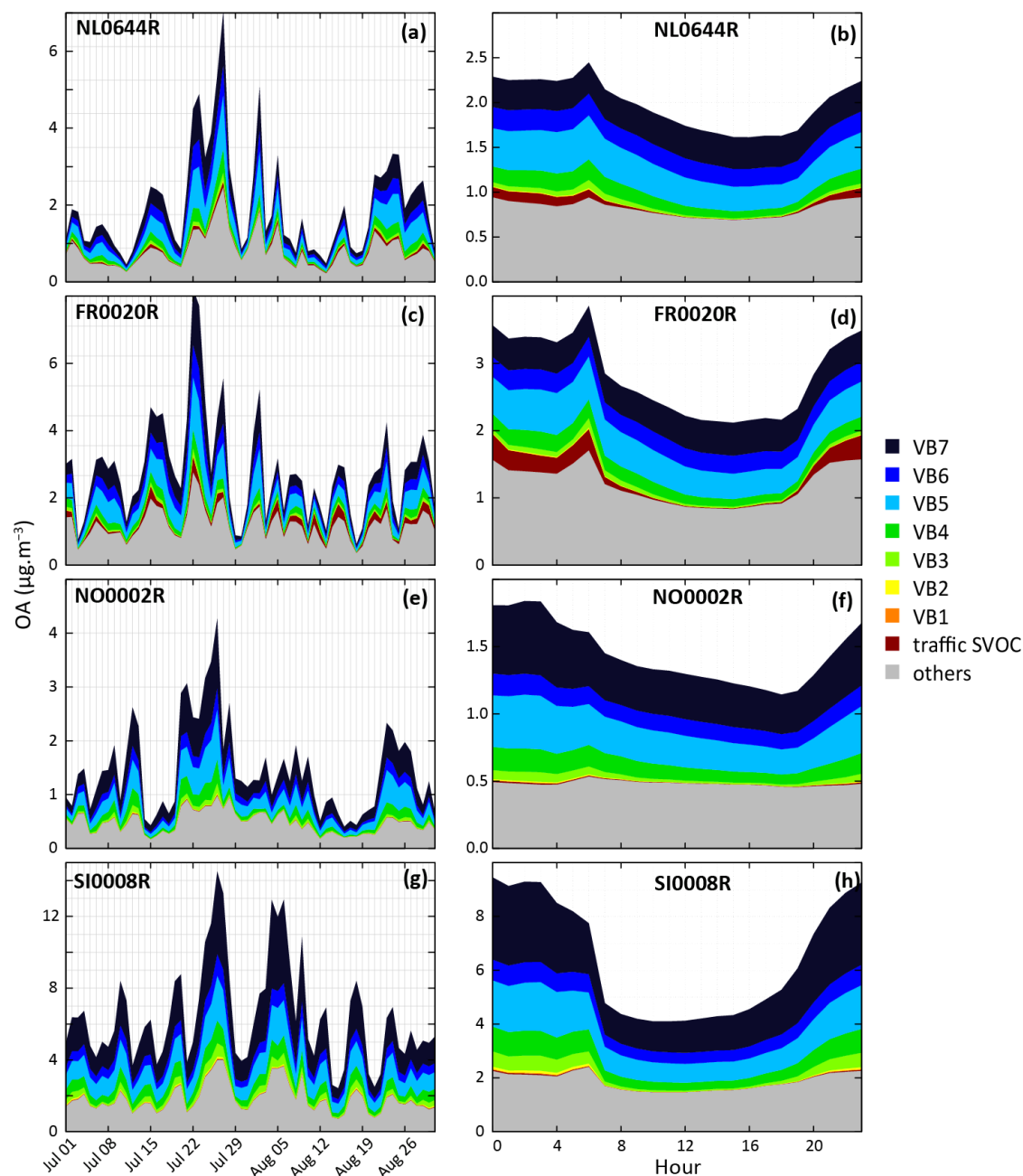


Figure S2 – Evolution of simulated OA concentrations and distribution function of volatility bins with the IVOC<sub>30VOC</sub> model configuration (from the less volatile one VB7, to the more volatile VB1). Panels b, d, f and h present mean daily profiles. Results are shown at two stations influenced by anthropogenic sources in Netherland (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<sub>14</sub> to C<sub>26</sub> emitted VBS-GECKO alkanes and alkenes and “others” includes all species from H<sub>2</sub>O mechanism.

5

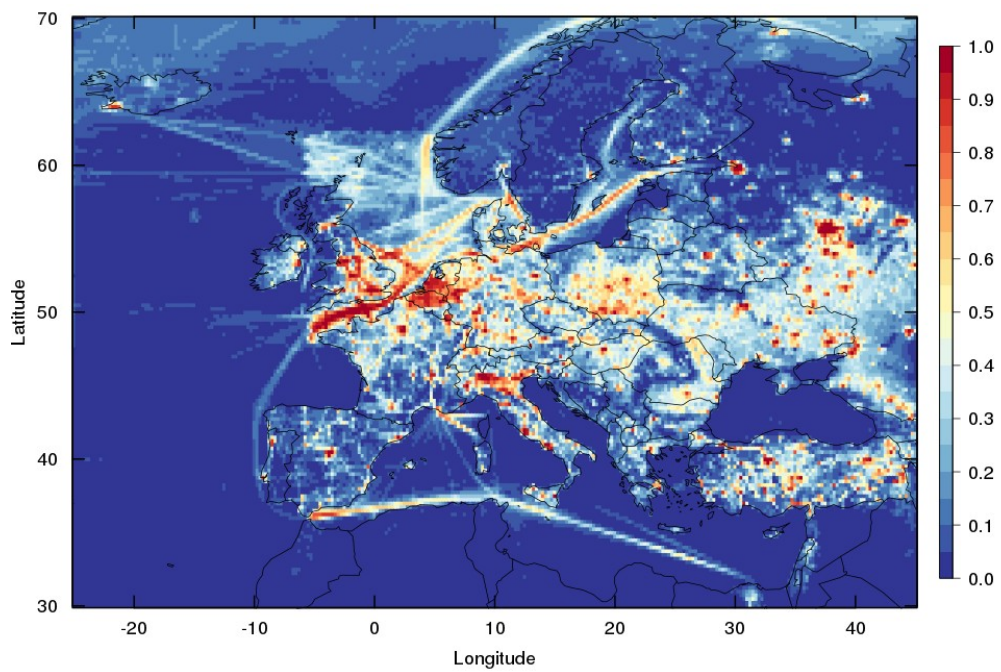


Figure S3 – Mean RRR over Europe during the two-month period for the ref-VBS-GECKO model configuration.