

Stadtler, S. et al.: Isoprene derived secondary organic aerosol in a global aerosol chemistry climate model

Supplement 2

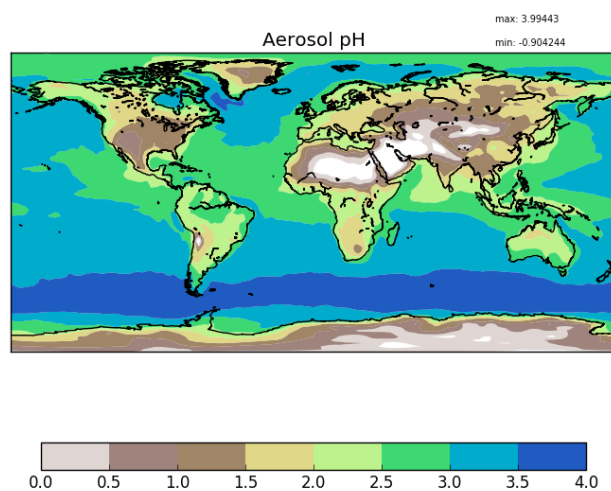


Figure S1: Aerosol pH values as calculated by AIM and used as input values in ECHAM-HAMMOZ to calculate IEPOX reaction probability.

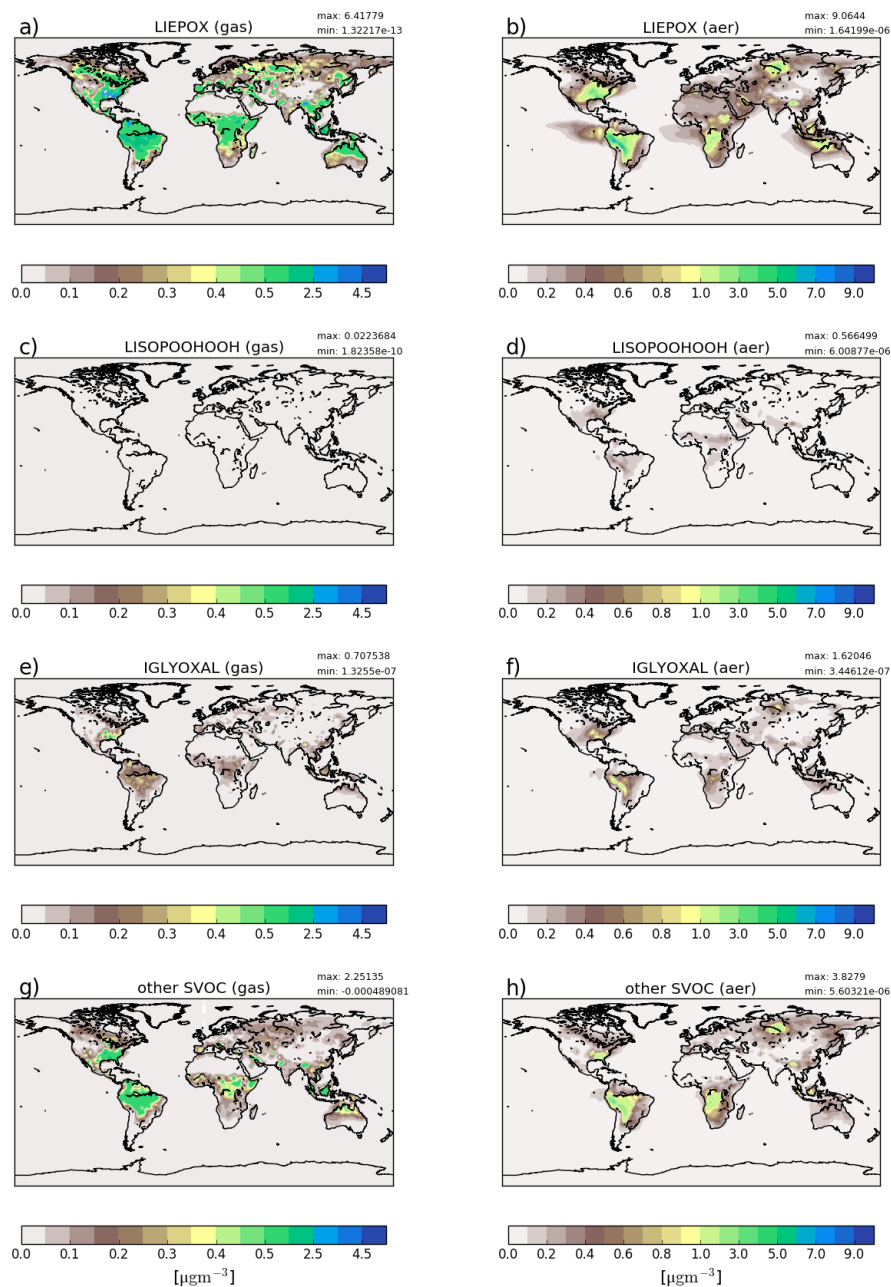


Figure S2: HshiftLC5 simulation average surface distribution of precursor gases (a, c, e, g) and corresponding component concentration in the particle phase (b, d, f, h) in $\mu g m^{-3}$ for June, July and August 2012. Different scales are used for precursors and iSOA to capture the concentration ranges accordingly. Note, that the concentration scales are not linear and focus on low concentrations.

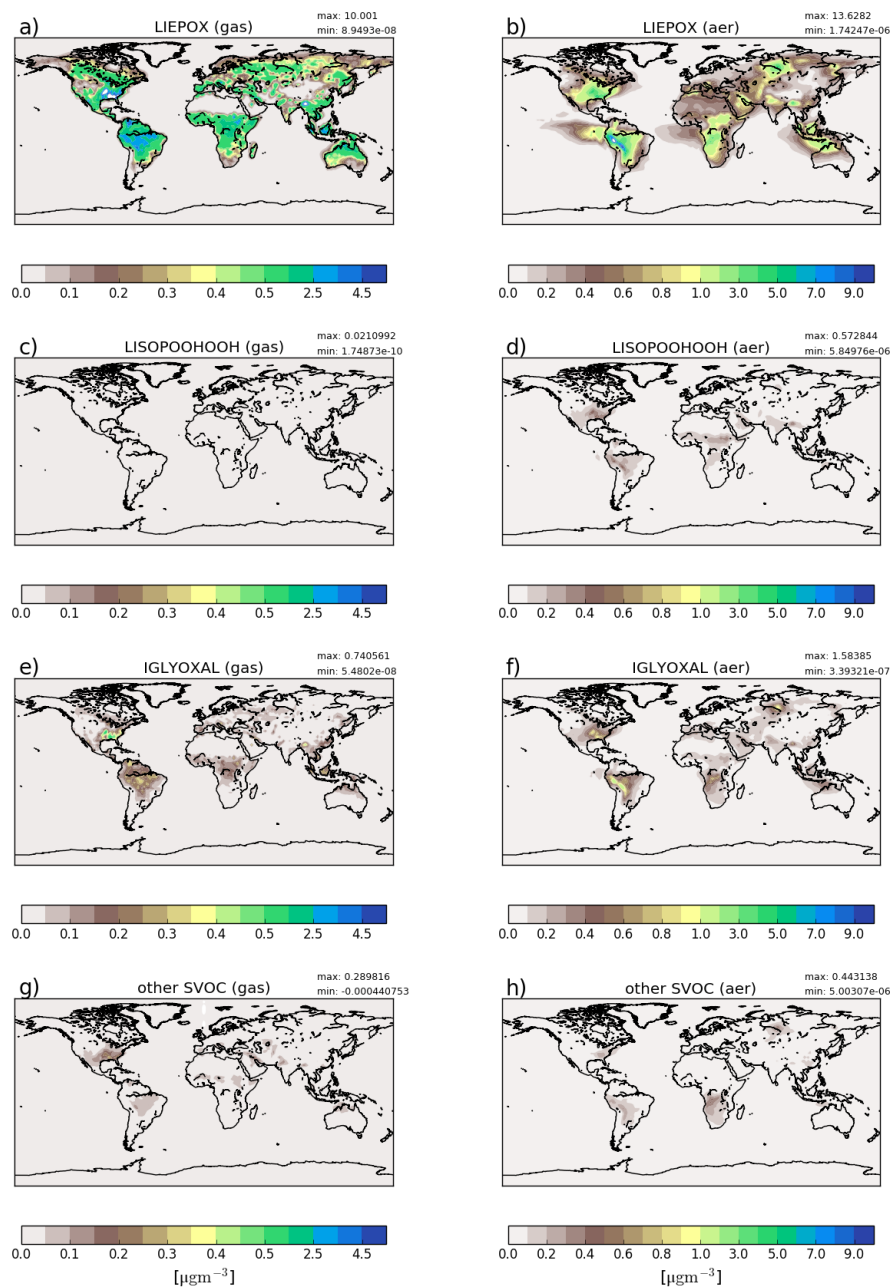


Figure S3: HshiftLIE simulation average surface distribution of precursor gases (a, c, e, g) and corresponding component concentration in the particle phase (b, d, f, h) in μgm^{-3} for June, July and August 2012. Different scales are used for precursors and iSOA to capture the concentration ranges accordingly. Note, that the concentration scales are not linear and focus on low concentrations.

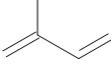
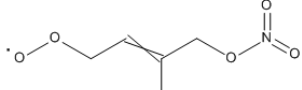
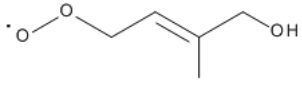
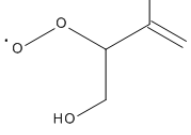
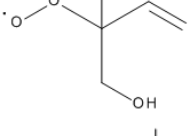
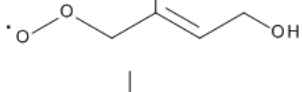
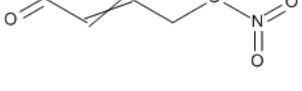
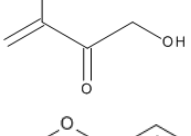

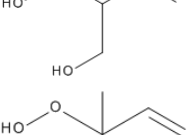
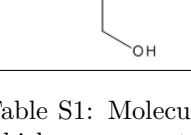
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|-------------------------------------------------------------------------------------|-----------------------------------|-------------------------------------|----------|
|  | <chem>C=CC(=C)C</chem> | C5H8 | C5H8 |
|  | <chem>[O]OCC=C(C)CON(=O)=O</chem> | NISOP02 | NISOP02 |
|  | <chem>[O]OC/C=C(/CO)C</chem> | LISOPACO2 (ISOP02 in Figure 1) | ISOPAO2 |
|  | <chem>OCC(O[O])C(=C)C</chem> | LISOPACO2 (ISOP02 in Figure 1) | ISOPDO2 |
|  | <chem>OCC(C)(O[O])C=C</chem> | ISOPBO2 (ISOP02 in Figure 1) | ISOPBO2 |
|  | <chem>[O]OC/C(=C/CO)/C</chem> | ISOPCO2 (ISOP02 in Figure 1) | ISOPCO2 |
|  | <chem>O=CC=C(C)CON(=O)=O</chem> | NC4CHO | NC4CHO |
|  | <chem>CC(=C)C(=O)CO</chem> | HCOC5 | HCOC5 |
|  | <chem>OOCC=C(C)CO</chem> | LISOPACOOH (ISOP00H in Figure 1) | ISOPAOOH |
|  | <chem>OCC(OO)C(=C)C</chem> | LISOPACOOH (ISOP00H in Figure 1) | ISOPDOOH |
|  | <chem>OCC(C)(OO)C=C</chem> | ISOPBOOH (ISOP00H in Figure 1) | ISOPBOOH |

Table S1: Molecular structures, SMILES codes, names in MOZ and in MCM, which are presented in Figure 1.

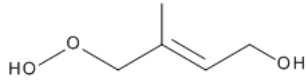
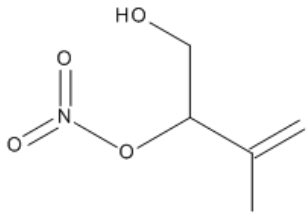
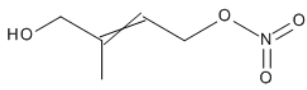
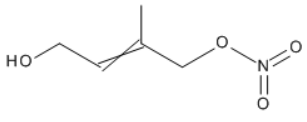
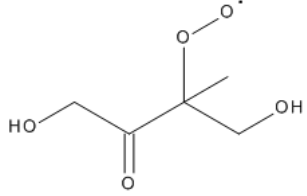
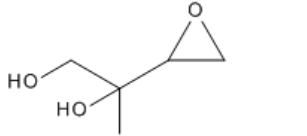
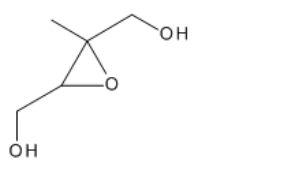
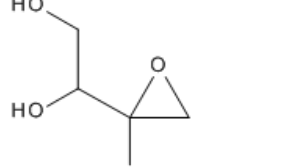
| Structure | SMILES | MOZ name | MCM name |
|-------------------------------------------------------------------------------------|----------------------------------|----------------------------------------|----------|
|  | <chem>OCC(=CCO)C</chem> | ISOPCOOH (ISOPOOH in Figure 1) | ISOPCOOH |
|  | <chem>OCC(ON(=O)=O)C(=C)C</chem> | ISOPDNO3 (ISOPNO3 in Figure 1) | ISOPDNO3 |
|  | <chem>OCC(=CCON(=O)=O)C</chem> | LISOPACNO3 (ISOPNO3 in Figure 1) | ISOPANO3 |
|  | <chem>OCC=C(C)CON(=O)=O</chem> | LISOPACNO3 (ISOPNO3 in Figure 1) | ISOPCNO3 |
|  | <chem>OCC(=O)C(C)(CO)O[O]</chem> | C59O2 | C59O2 |
|  | <chem>CC(O)(CO)C1CO1</chem> | LIEPOX | IEPOXA |
|  | <chem>OCC1OC1(C)CO</chem> | LIEPOX | IEPOXB |
|  | <chem>CC1(CO1)C(O)CO</chem> | LIEPOX | IEPOXC |

Table S2: Continued: Molecular structures, SMILES codes, names in MOZ and in MCM, which are presented in Figure 1.

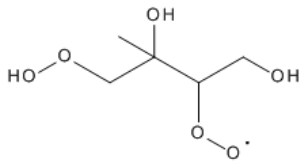
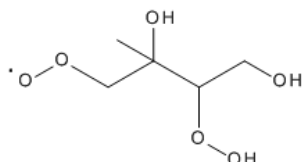
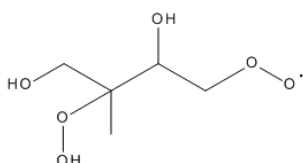
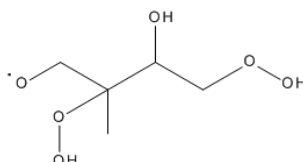
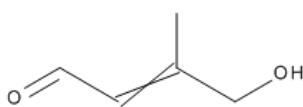
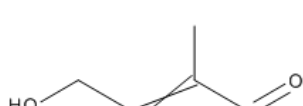
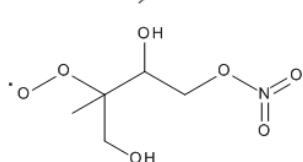
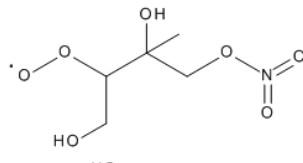
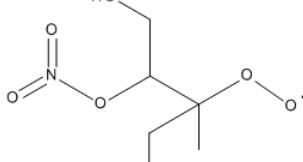
| Structure | SMILES | MOZ name | MCM name |
|-------------------------------------------------------------------------------------|----------------------------------------|------------|----------|
|  | <chem>CC(O)(COO)C(CO)O[O]</chem> | LISOPOOHO2 | — |
|  | <chem>CC(O)(CO[O])C(CO)OO</chem> | LISOPOOHO2 | — |
|  | <chem>CC(CO)(OO)C(O)CO[O]</chem> | LISOPOOHO2 | — |
|  | <chem>CC(C[O])(OO)C(O)COO</chem> | LISOPOOHO2 | — |
|  | <chem>CC(=CC=O)CO</chem> | LHC4ACCHO | HC4ACHO |
|  | <chem>CC(=CCO)C=O</chem> | LHC4ACCHO | HC4CCHO |
|  | <chem>OCC(C)(O[O])C(O)CON(=O)=O</chem> | LISOPNO3O2 | INAO2 |
|  | <chem>OCC(O[O])C(C)(O)CON(=O)=O</chem> | LISOPNO3O2 | INCO2 |
|  | <chem>OCC(ON(=O)=O)C(C)(CO)O[O]</chem> | LISOPNO3O2 | INDO2 |

Table S3: Continued: Molecular structures, SMILES codes, names in MOZ and in MCM, which are presented in Figure 1.

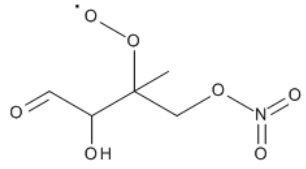
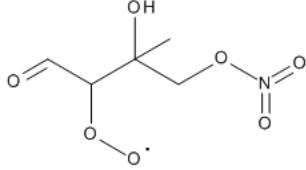
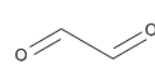
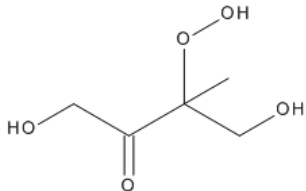
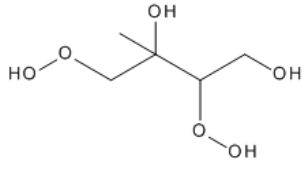
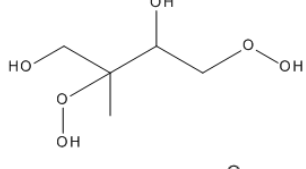
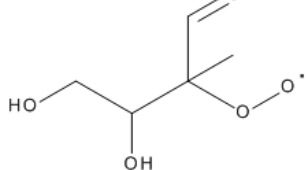
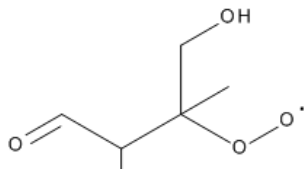
| Structure | SMILES | MOZ name | MCM name |
|-------------------------------------------------------------------------------------|-----------------------------------------|-------------|----------|
|  | <chem>O=CC(O)C(C)(O[O])CON(=O)=O</chem> | LNISO3 | C510O2 |
|  | <chem>CC(O)(CON(=O)=O)C(O[O])C=O</chem> | LNISO3 | — |
|  | <chem>O=CC=O</chem> | IGLYOXAL | GLYOX |
|  | <chem>OCC(=O)C(C)(CO)OO</chem> | C59OOH | C59OOH |
|  | <chem>CC(O)(COO)C(CO)OO</chem> | LISOPOOHOOH | — |
|  | <chem>CC(CO)(OO)C(O)COO</chem> | LISOPOOHOOH | — |
|  | <chem>OCC(O)C(C)(O[O])C=O</chem> | LC578O2 | C57O2 |
|  | <chem>O=CC(O)C(C)(CO)O[O]</chem> | LC578O2 | C58O2 |

Table S4: Continued: Molecular structures, SMILES codes, names in MOZ and in MCM, which are presented in Figure 1.

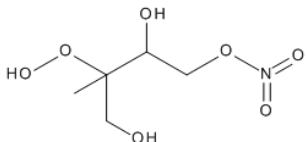
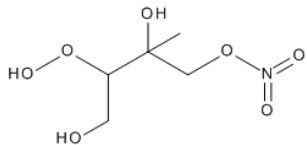
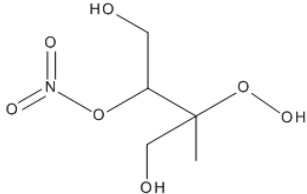
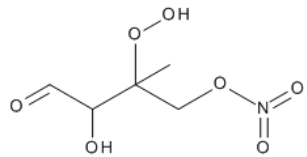
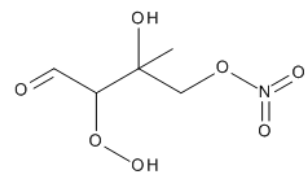
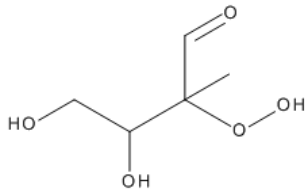
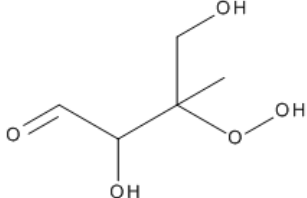
| Structure | SMILES | MOZ name | MCM name |
|-------------------------------------------------------------------------------------|---------------------------------------|--------------|----------|
|  | <chem>OCC(C)(OO)C(O)CON(=O)=O</chem> | LISOPNPO3OOH | INAOOH |
|  | <chem>OCC(OO)C(C)(O)CON(=O)=O</chem> | LISOPNPO3OOH | INAOOH |
|  | <chem>OCC(ON(=O)=O)C(C)(CO)OO</chem> | LISOPNPO3OOH | INDOOH |
|  | <chem>O=CC(O)C(C)(OO)CON(=O)=O</chem> | LNISOOH | C510OOH |
|  | <chem>CC(O)(CON(=O)=O)C(OO)C=O</chem> | LNISOOH | — |
|  | <chem>OCC(O)C(C)(OO)C=O</chem> | LC578OOH | C57OOH |
|  | <chem>O=CC(O)C(C)(CO)OO</chem> | LC578OOH | C58OOH |

Table S5: Continued: Molecular structures, SMILES codes, names in MOZ and in MCM, which are presented in Figure 1.