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Simulation of organic aerosol, its precursors, and related oxidants in the Landes pine forest in southwestern France: accounting for domain-specific land use and physical conditions

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Supplementary information

S1: Three domains used for the study (Figure S1)

Figure S1: Domains used in the study: 1: European coarse domain (25kmx25km horizontal resolution), 2: French intermediate domain (5kmx5km horizontal resolution) and 3: high-resolution domain (1kmx1km horizontal resolution. © OpenStreetMap contributors 2022. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

S2: Meteorological tests

Tests with eight different set-ups of meteorological models or model data were performed in order to choose the two used in the article, seven of them using WRF with different parametrizations and the last one with ECMWF high-resolution forecast fields. Out of the seven parametrizations tested for WRF three had convergence/stability issues, therefore they were not compared to the data, the remaining four resulted in complete simulations for all the three domains. The characteristics of these simulations are indicated in Table SI1. The meteorological fields for each domain were tested against E-OBS data and output for the high-resolution domain (1 km horizontal resolution) was compared to in-situ meteorological measurements at Bilos, France. The results for the comparisons for the smallest domain were provided in the main article, the results for the rest of the comparisons will be provided here (Table SI1 and SI2). The WRF simulation chosen as a result of this comparison is noted here as WRF3. Simulations WRF5 through WRF7 had convergence/stability issues.

Table SI2 shows that for the coarse domain (Europe) and also the intermediary domain (France) the correlation of the ECMWF data is better with the EOBS data regardless of the type of temperature variable or the domain; the bias however seems to be less in the WRF 3 simulations. The correlation comparisons for the rest of the presented variables (wind speed, wind direction and relative humidity) show all the same results: ECMWF seems to better correlate with observations; contrary to the temperature variables the bias for these three parameters is lowest for ECMWF for both domains.

Table S1: Information about parameterizations used for the WRF simulations. The last three had convergence/instability issues, the first four resulted in complete simulations for all three domains. Statistical data for the comparisons of these parameterizations to E-OBS data are given in table SI2. The numbers in the table indicate the parametrization number that is used for a specific parametrization the WRF configuration file; these numbers can be checked by looking the parameter up in the WRF documentation (Wang et al, 2015).

Case:	WRF1	WRF2	WRF3	WRF4	WRF5	WRF6	WRF7
sf_sfclay_physics	1	1	5	1	1	5	5
sf_surface_physics	1	4	4	2	2	2	3
bl_pbl_physics	1	1	6	1	1	6	6
cu_physics	1	1	1	1	1	1	1
ra_lw_physics	1	1	4	4	1	4	4
ra_sw_physics	1	1	4	4	1	4	4
mp_physics	3	6	6	6	6	6	6
icloud	1	1	1	1	1	1	1
ifsnow	0	0	0	0	0	0	0
sf_urban_physics	0	0	1	0	1	1	1
feedback	1	1	1	1	1	1	1
diff_opt	1	1	1	1	1	1	1
diff_6th_opt	0	0	0	0	0	0	0
sst_update	0	0	1	1	0	1	1
sf_lake_physics	1	1	1	1	1	1	1
topo_wind	0	0	1	1	0	1	1
sf_surface_mosaic	0	0	0	0	0	1	0
mosaic_lu	0	0	0	0	0	0	1

mosaic_soil	0	0	0	0	0	0	1
isfflx	1	1	1	1	1	1	1
grid_fdda	0	0	2	1	0	1	1
dveg	0	0	2	4	0	4	4

Table S2: Statistics for all the meteorologic runs, R is the correlation, B the bias, M the average and SD the standard deviation. The statistics are in °C for temperature, m/s for wind speed, and degrees for wind direction. The parameterizations for each WRF run are given in table SI1. According to these results as well as the comparisons for the measurement site for the finest domain, WRF3 was chosen since it represents the lowest bias and the highest correlation for most parameters.

				EUR25						***SFRA5***			
		WRF 1	**WRF 2**	**WRF 3**	**WRF 4**	**ECMWF**	**E-Obs**	**WRF 1**	**WRF 2**	**WRF 3**	**WRF 4**	**ECMWF**	**E-Obs**
Min temp	R	0,76	0,75	0,73	0,72	0,83		0,82	0,82	0,79	0,79	0,91	
	B	0,64	0,95	0,01	0,33	-0,74		0,52	1,05	-0,31	-0,07	-1,18	
	M	10,71	10,39	11,34	11,01	12,09	11,34	12,82	12,21	13,77	13,60	14,57	13,54
	SD	2,41	2,54	2,59	2,49	2,21	2,69	2,80	3,01	3,23	3,20	2,73	2,92
Mean temp	R	0,87	0,86	0,88	0,86	0,94		0,93	0,91	0,94	0,94	0,97	
	B	1,03	1,20	0,06	0,43	0,56		1,67	1,71	-0,31	0,03	0,15	
	M	14,62	14,45	15,59	15,22	15,09	15,65	17,54	17,55	19,70	19,36	19,09	19,42
	SD	2,31	2,29	2,56	2,42	2,35	2,51	2,60	2,78	3,28	3,26	3,19	3,25
Max temp	R	0,82	0,80	0,83	0,81	0,90		0,91	0,88	0,91	0,92	0,97	
	B	2,37	2,70	1,12	1,56	2,15		3,43	3,34	0,52	0,93	1,84	
	M	18,98	18,65	20,22	19,78	19,19	21,34	21,68	21,91	24,90	24,39	23,55	25,69
	SD	2,70	2,63	3,02	2,89	3,05	3,38	2,82	3,03	3,82	3,69	4,15	4,32
Wind speed	R	0,70	0,70	0,69	0,66	0,82		0,78	0,78	0,77	0,76	0,92	
	B	0,13	-0,12	-0,37	-0,26	0,07		0,41	0,26	0,42	0,45	0,32	
	M	3,26	3,52	3,77	3,66	3,32	3,39	2,80	3,01	2,80	2,76	2,79	3,19
	SD	1,56	1,66	1,81	1,75	1,29	1,29	1,35	1,46	1,33	1,36	1,10	1,16
Wind direction	R	0,53	0,53	0,54	0,52	0,64		0,33	0,34	0,33	0,29	0,42	
	B	-8,35	-8,00	-2,52	-4,40	-1,16		5,59	7,24	2,35	3,62	16,89	
	M	210,08	209,73	204,24	206,12	202,88	201,72	213,72	215,22	225,62	218,79	211,73	235,48
	SD	84,71	84,38	87,17	86,02	66,63	86,24	109,55	107,81	105,87	113,22	71,70	106,63

Relative humidity	R	0,64	0,61	0,69	0,66	0,88		0,50	0,49	0,67	0,69	0,89	
	B	-8,83	-8,42	-0,50	-1,61	1,78		-13,31	-11,85	1,68	0,17	4,12	
	M	79,27	78,86	70,94	72,05	68,66	70,44	83,12	81,14	66,80	68,56	63,76	68,00
	SD	8,71	7,34	8,85	8,66	9,50	10,20	5,97	4,48	8,19	7,60	8,89	9,26

S3: Bowen ratio, precipitation and ozone deposition speed comparisons

The Bowen ratio (ratio of sensible to latent heat fluxes at the surface) and precipitation comparisons are shown in figure SI2, while ozone deposition comparisons are shown in figure SI3. Precipitation periods and episodes are quite well represented by the model, while the precipitation intensity is underestimated. The Bowen ratio is also well simulated by the model, missing some extreme values during precipitation episodes which could be related to the underestimation of the precipitation intensity. The ozone deposition velocity also corresponds roughly to observations, therefore we conclude that the nighttime ozone overestimation in the simulations should not be related to an underestimation of ozone deposition.

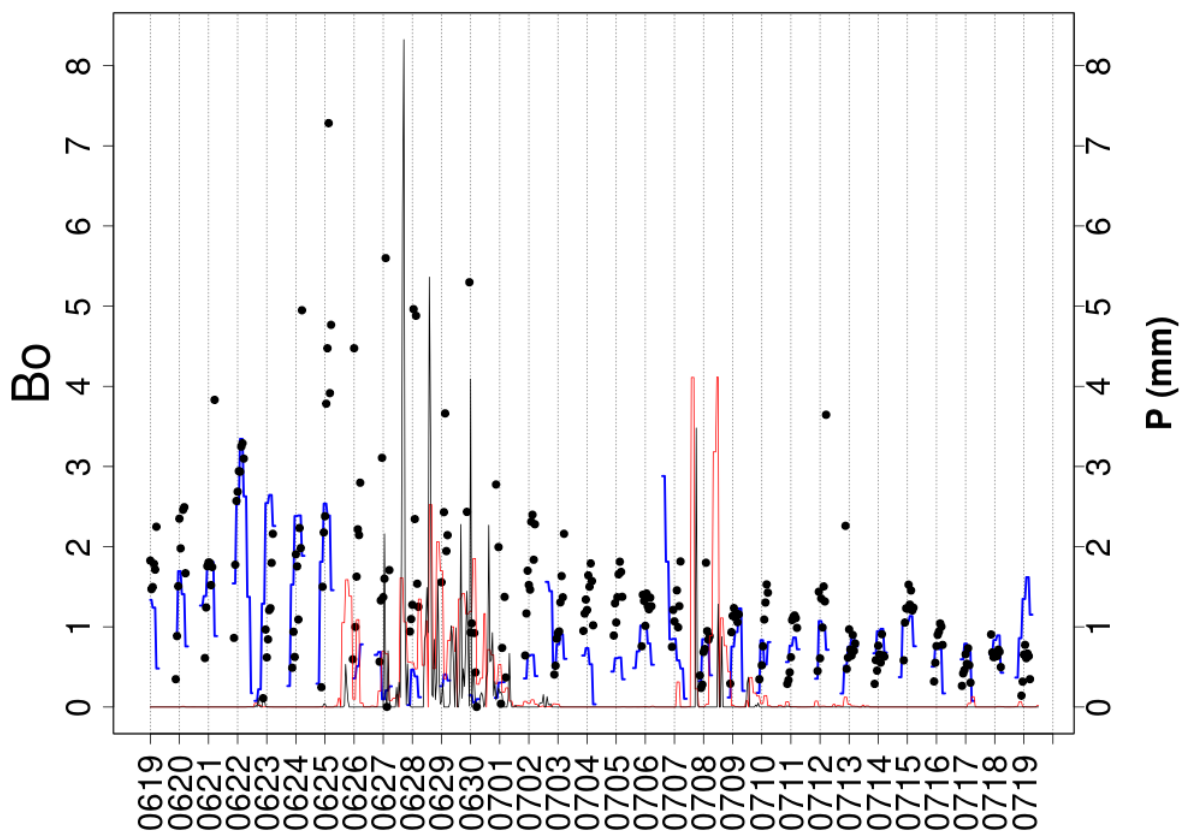

Figure S2: Bowen ratio (left axis) and precipitation comparisons for the Bilos site. Precipitation (red for model, black lines for observations) and Bowen ratio (blue for model and black dots for observations) are shown here.

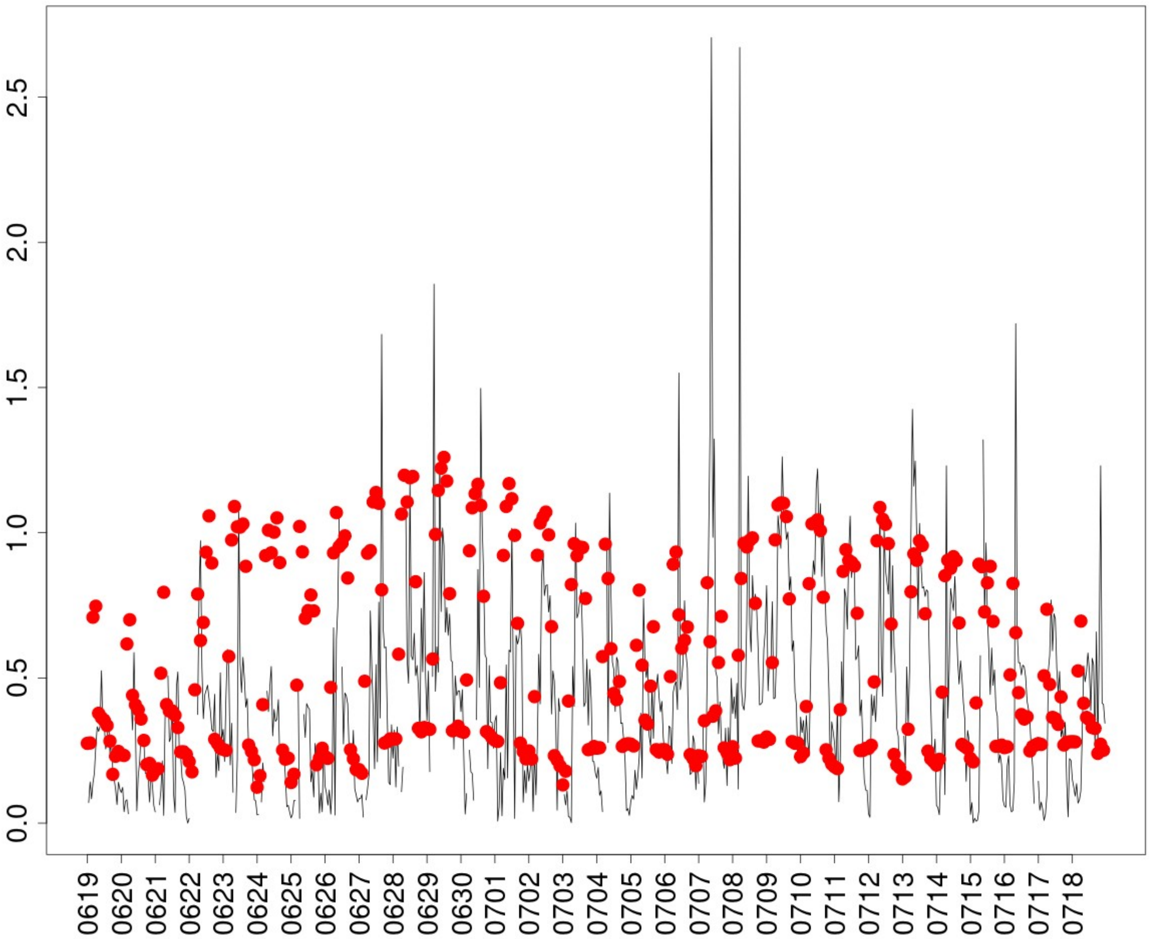

Figure S3 : Deposition speed (m/s) comparisons for ozone : black lines show the measurements and red dots simulations. The temporal resolution for the measurements is hourly, while simulations have a bi-hourly frequency.

S4: Anthropogenic emissions

The high-resolution anthropogenic emissions were taken from Atmo-NA, they were processed in a R module prepared for the purpose and mimicking some of the functionalities of EmiSurf (the anthropogenic emissions pre-processor for the CHIMERE model) There emissions were compared with the EMEP emissions for the same year. The reference year in these comparisons is the 2014. The emissions for EMEP database did not show a significant change between 2014 to 2017 (to be verified here: https://www.ceip.at/webdab-emission-database/emissions-as-used-in-emep-models). For the simulations, the 2014 Atmo-NA emissions were used. In this section, only a minimal comparison for a short list of species will be shown (Figures SI3 to SI5) and the general statistical comparisons for all the species will be shown in Table SI2.

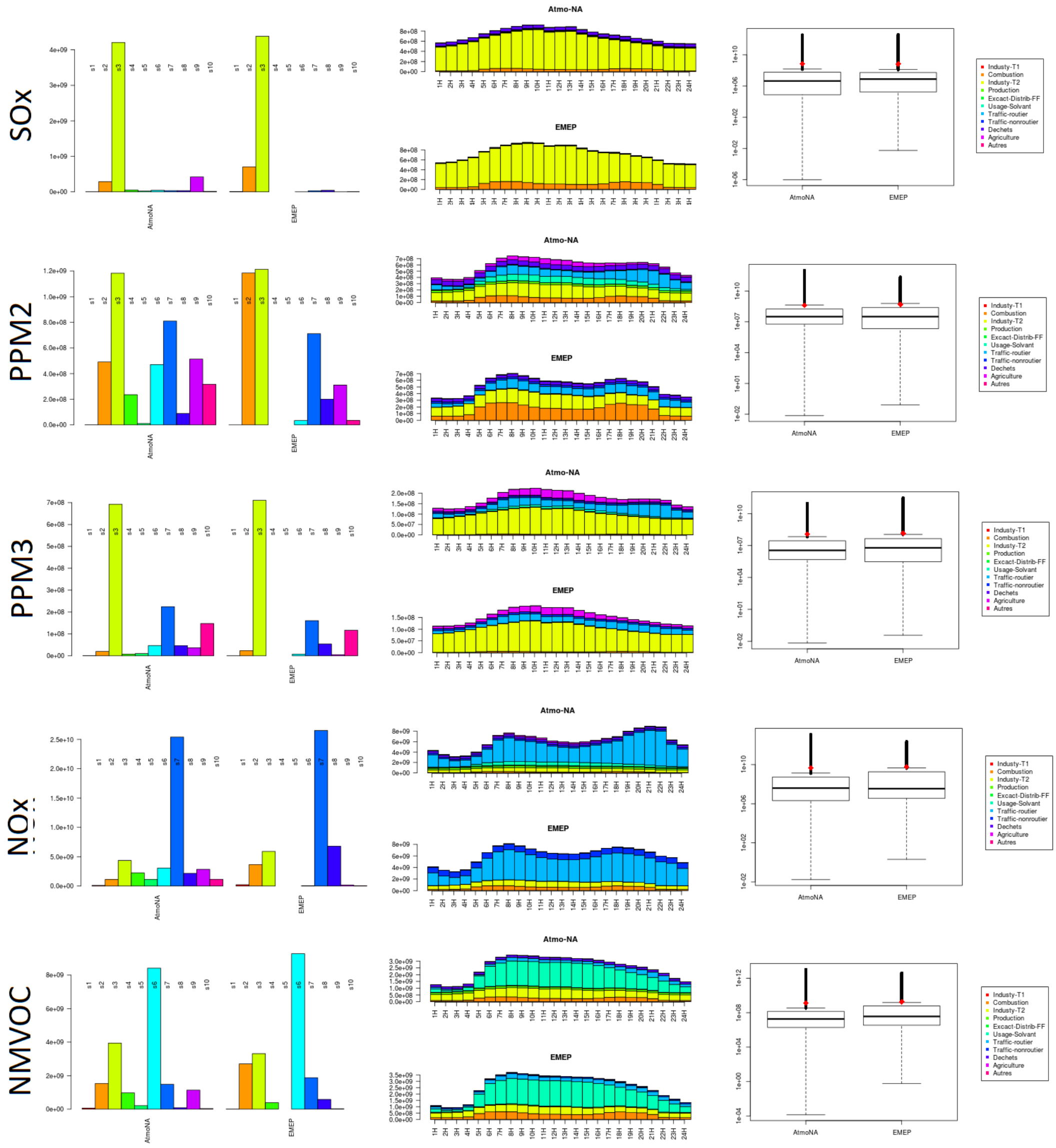

Figure S4: Figure S4: Comparisons for the emissions in Atmo-NA and EMEP for different grouped species for the month of June. For each species (a row per species) total emission boxplot comparisons are shown on right, snap sector barplot comparisons on the left and daily profile of snap sectors in the middle. All the values are shown in molecules/cm2/s . Comparisons are performed over the fine simulation domain. For clarity, PPM2 and PPM3 from the EMEP emissions inventory indicate the fine and coarse portions of the emitted aerosols respectively.

Table S3 : Comparison between Atmo-NA and EMEP emissions for the month of June and July and the dominant sector in both inventories for grouped species.

Grouped species	**Bias (AtmoNAEMEP)/EMEP*100**	**Dominant sector (Atmo-NA)**	**Dominant sector (EMEP)**
CO	-0.46 %	Snap2 (Non-industrial combustion)	Snap2 (Non-industrial combustion)
NO_x	+4.16 %	Snap7 (Road trafic)	Snap7 (Road trafic)
SO_x	+22.2 %	Snap3 (Production industry combustion)	Snap3 (Production industry combustion)
NMVOC	+4 %	Snap 6 (Solvent use)	Snap 6 (Solvent use)
NH_3	+3.7 %	Snap10 (Agriculture)	Snap10 (Agriculture)
PM_{10}	+16.2 %	Snap3 (Production industry combustion)	Snap3 (Production industry combustion)
$PM_{2.5}$	+16.3 %	Snap3 (Production industry combustion)	Snap3 (Production industry combustion)

S5: NO_2 comparisons

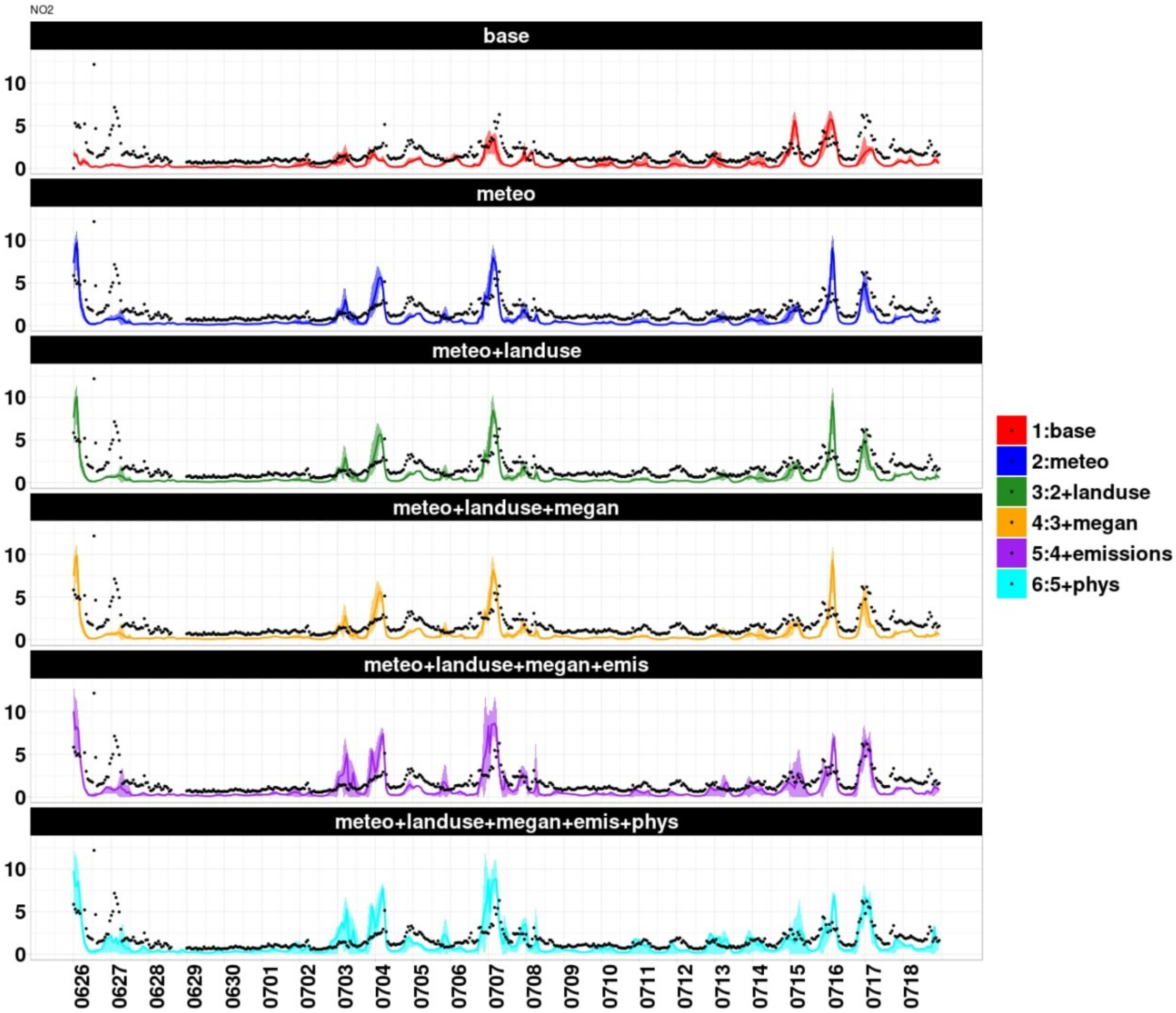

Figure S5 : Comparisons for NO_2. All values are shown in ppb.

S6: More detailed BVOC comparisons

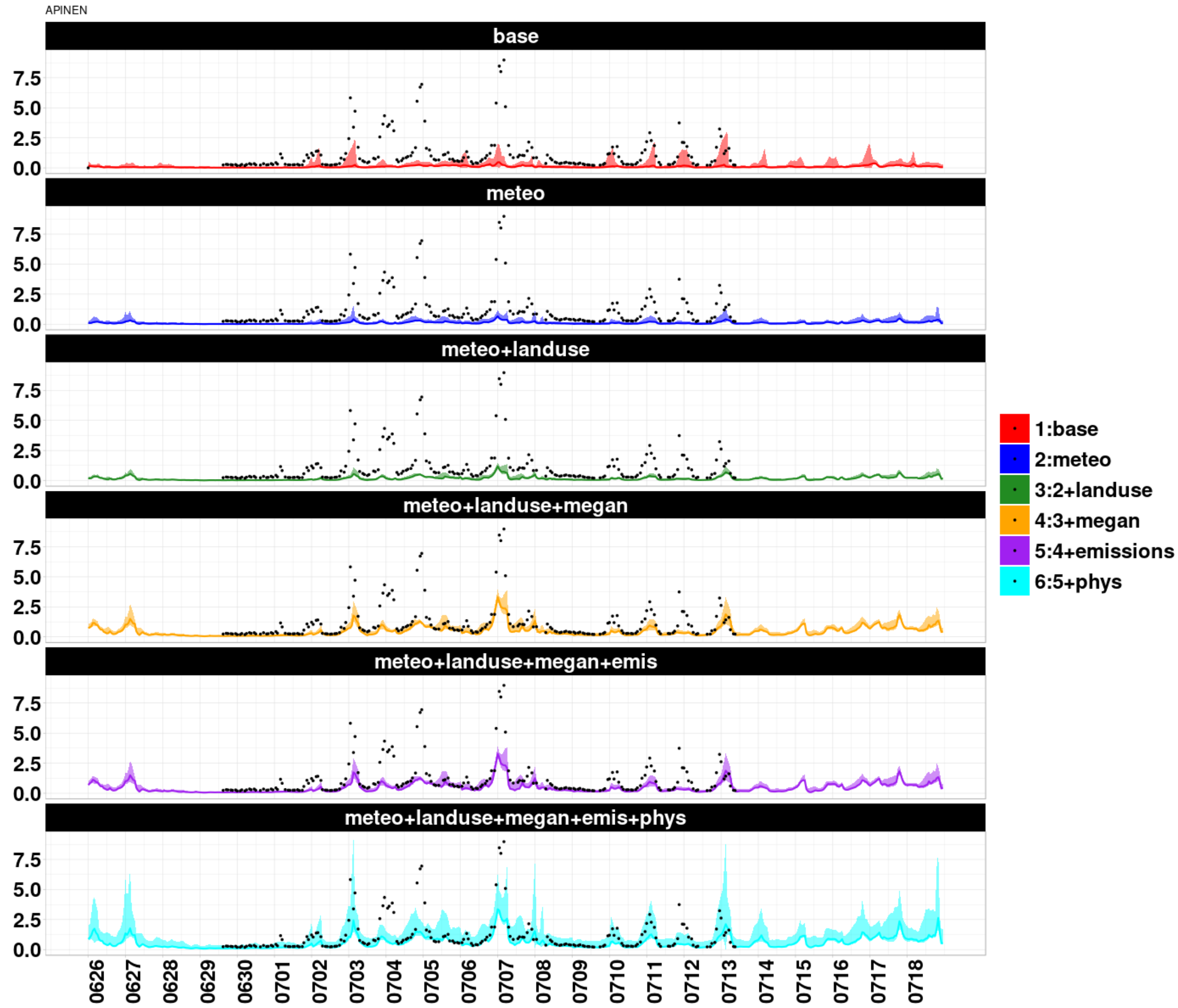

Figure S6: Comparisons for a-pinene, all data is shown in ppb.

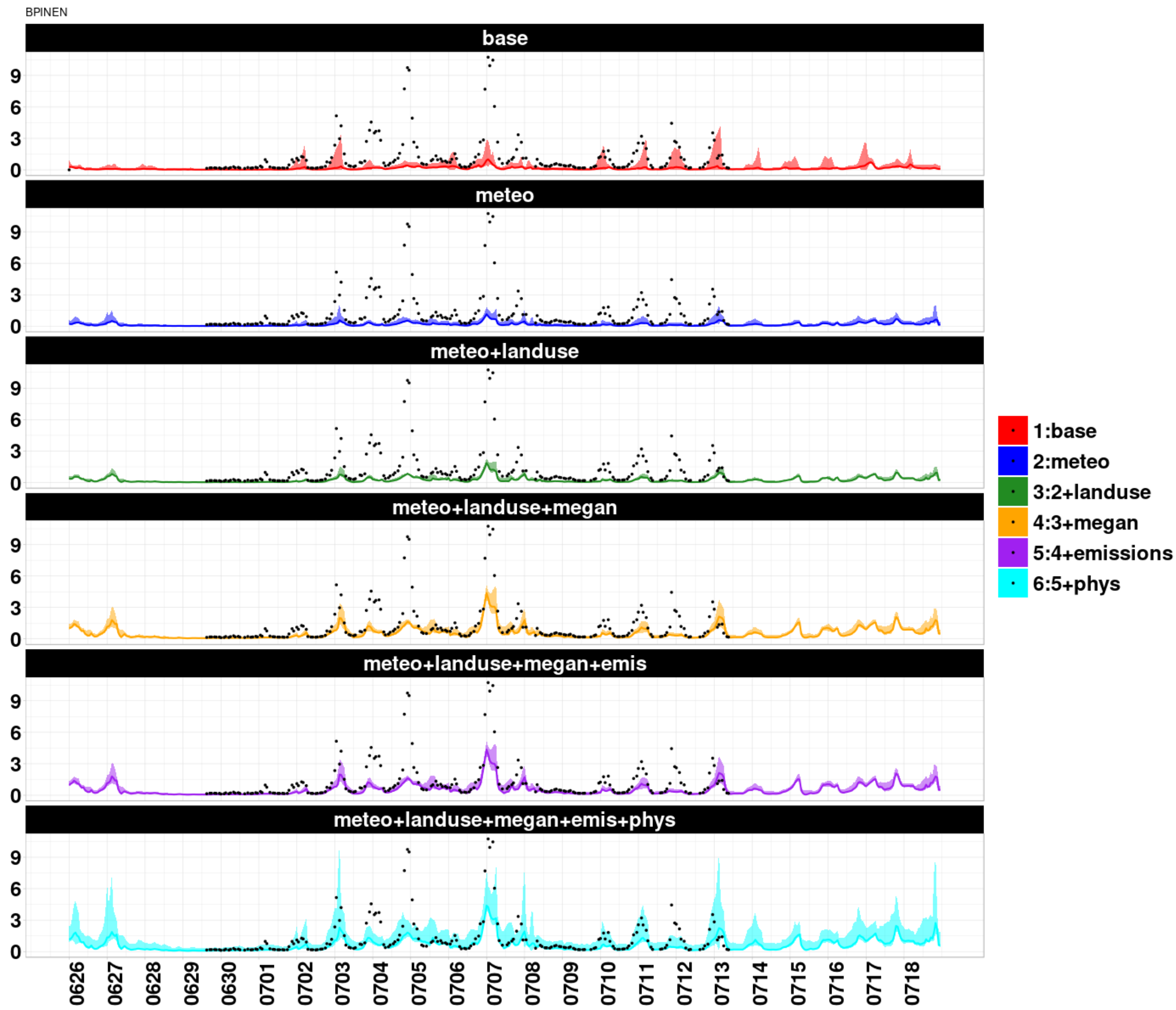

Figure S7: Comparisons for b-pinene, all data is shown in ppb.

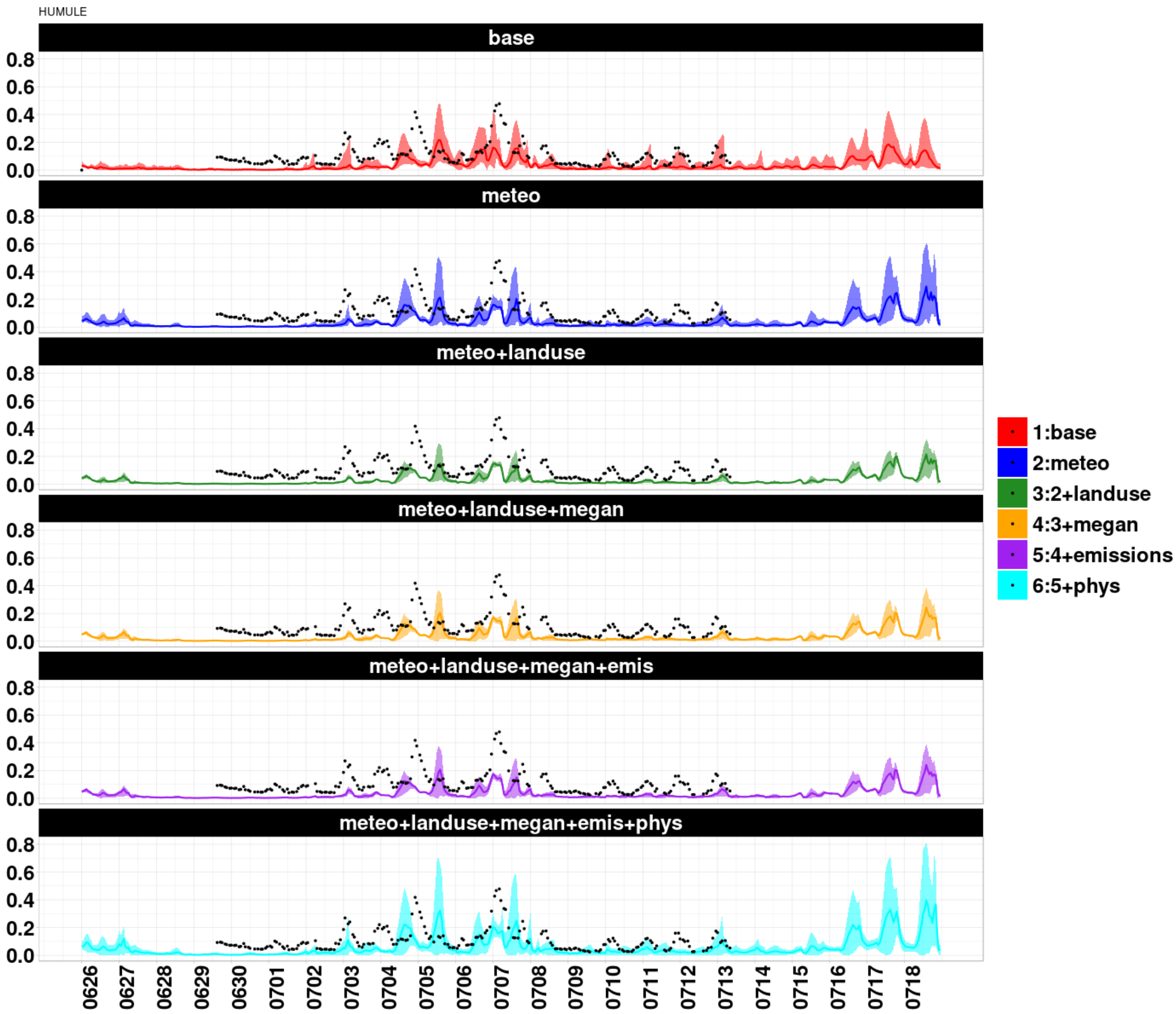

Figure S8: Comparisons for humulene, all data is shown in ppb.

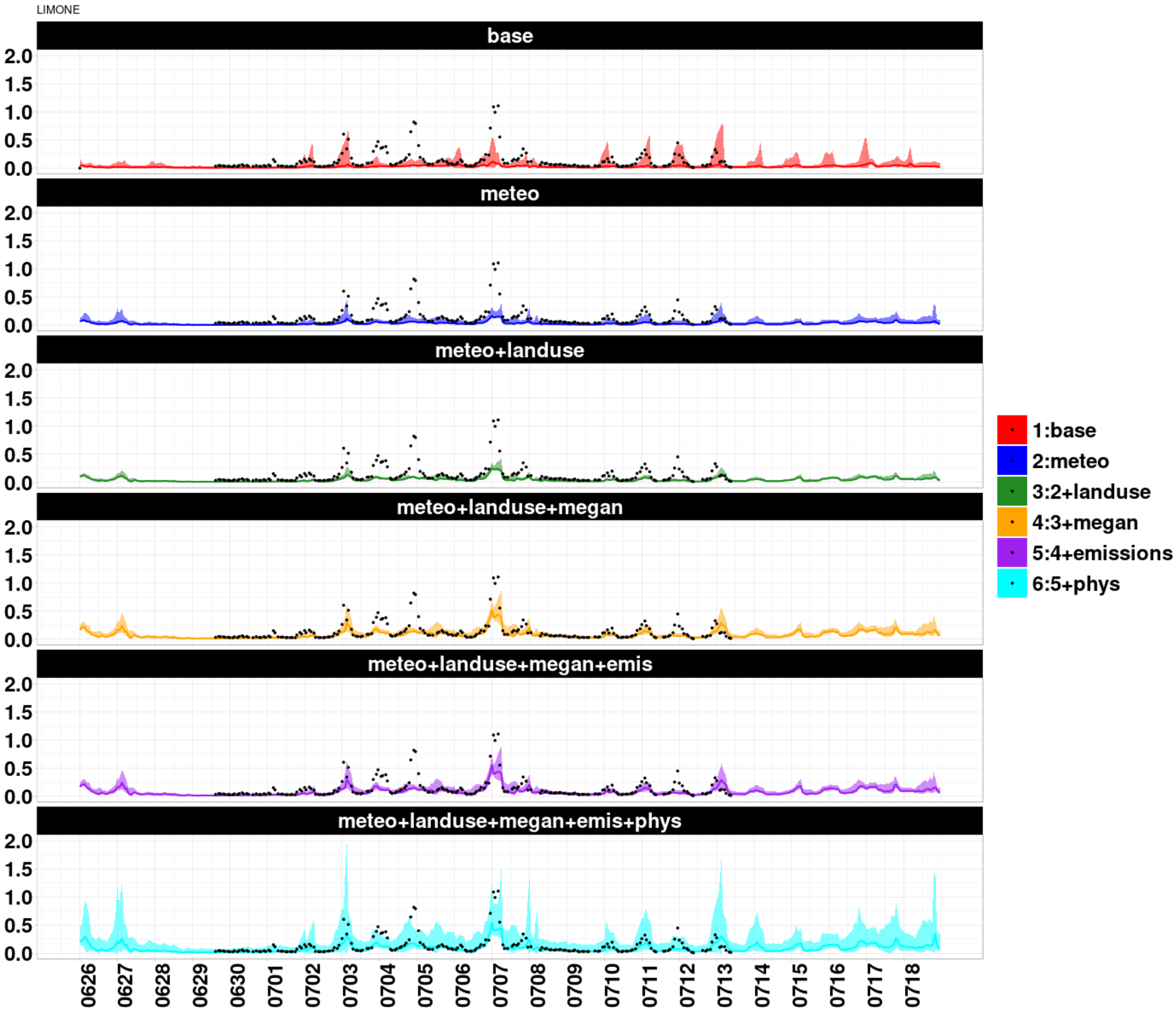

Figure S9: Comparisons for limonene, all data is shown in ppb.

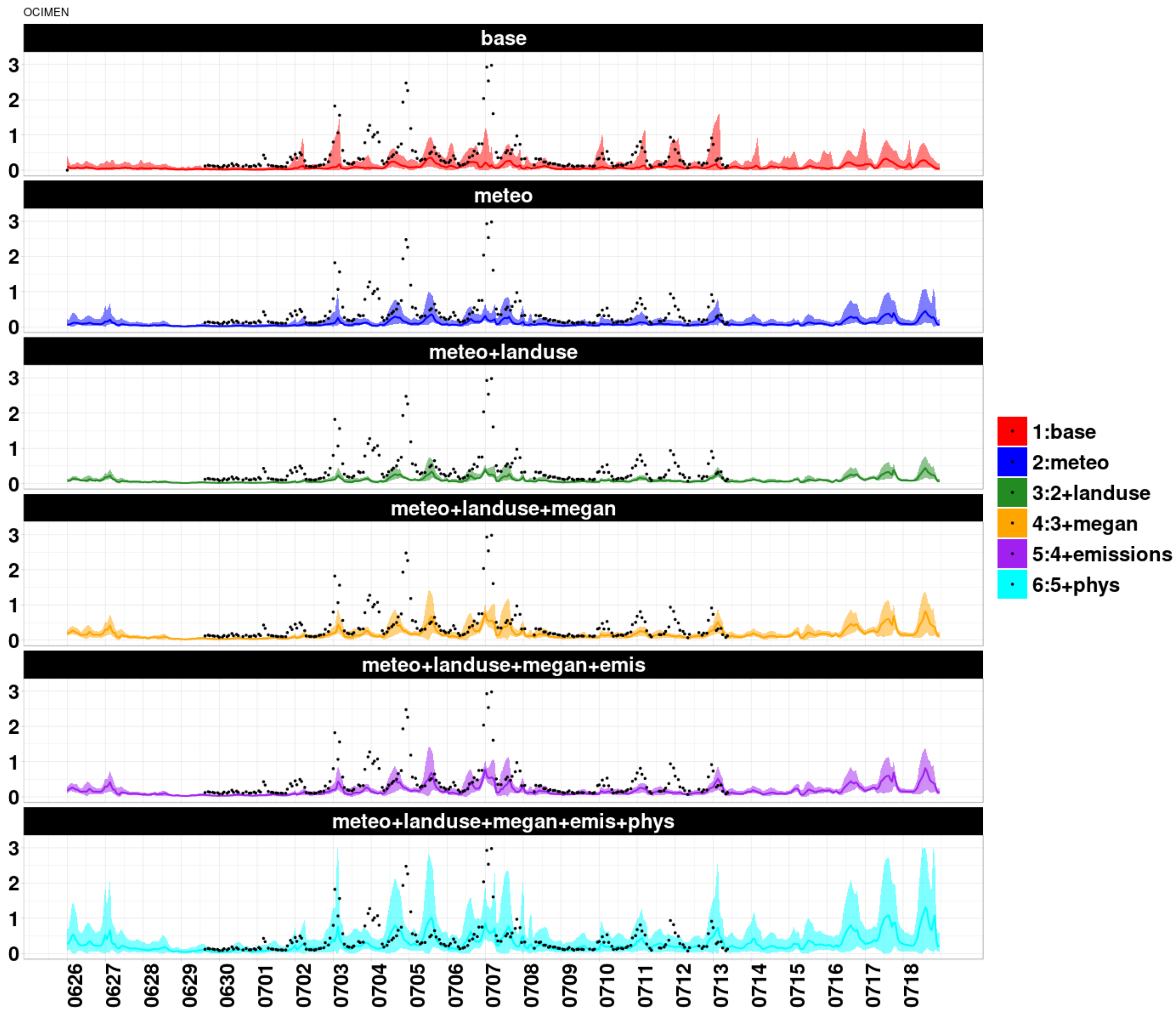

Figure S10: Comparisons for the sum of ocimene and myrcene, all data is shown in ppb.

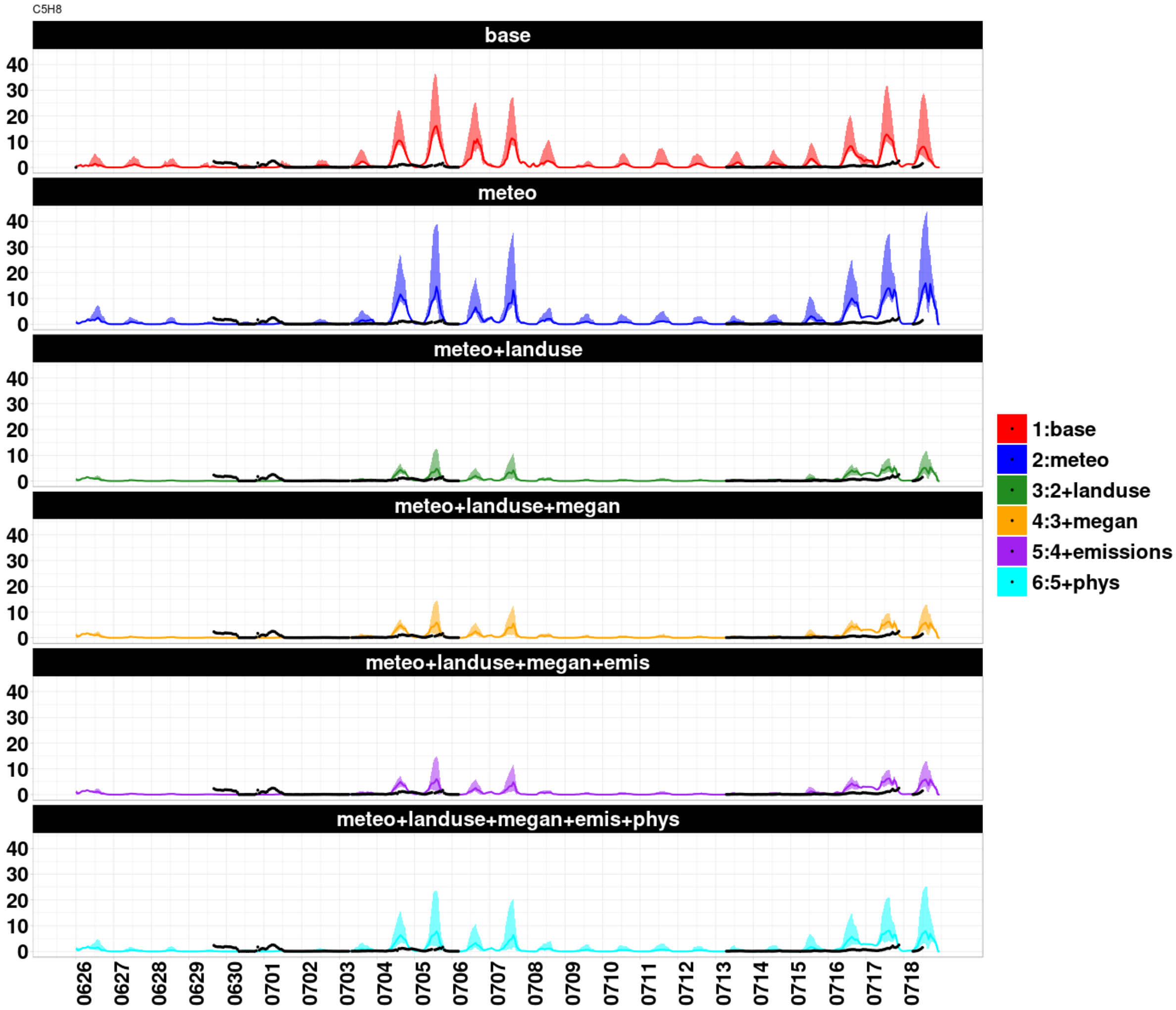

Figure S11: Comparisons for isoprene, all data is shown in ppb.

S7: Animations

GIFs for several species can be downloaded in the following address: https://drive.google.com/drive/folders/1LaRMgb_9ZYvb1SsWWdpd28kYBP2ajywl?usp=sharing

For each species, 2 maps are shown, one with the initial model configuration (on the left) and one after having implemented all modifications (on the right). The figures regard to the finest domain of the simulations. All figures are shown in ppb, except pBSOA (particulate BSOA), PM2.5 which is shown in µg.m^{-3}, rh in a scale of 0/1 and temp in K.

S8: BVOC reactions

The following reactions show the gas-phase formation of BSOA species from the oxidation of BVOCs. The surrogate SOA compounds consist of six hydrophilic species that include an anthropogenic nondissociative species (AnA0D), an anthropogenic once-dissociative species (AnA1D), an anthropogenic twice-dissociative species (AnA2D), a biogenic non dissociative species (BiA0D), a biogenic once-dissociative species (BiA1D) and a biogenic twice-dissociative species (BiA2D), three hydrophobic species that include an anthropogenic species with moderate saturation vapor pressure (AnBmP), an anthropogenic species with low saturation vapor pressure (AnBlP) and a biogenic species with moderate saturation vapor pressure (BiBmP), and two surrogate compounds for the isoprene oxidation products. BiSQT is the surrogate species formed from the oxidation of sesqui-terpenes, ISOPA1 and ISOPA2 are the oxidation products of isoprene. The reaction constants are given in molec.$cm^{-3}.s^{-1}$.

Isoprene with OH:

C5H8+OH->0.232*ISOPA1+0.0288*ISOPA2+... k(T)=Aexp(-B/T),A=2.54e-11,B=-410

OH reactions:

APINEN+OH->0.30*BiA0D+0.17*BiA1D+0.10*BiA2D+... k(T)=Aexp(-B/T),A=1.87e-11,B=-435

BPINEN+OH->0.07*BiA0D+0.08*BiA1D+0.06*BiA2D+... k(T)=Aexp(-B/T),A=2.38e-11,B=-357

OCIMEN+OH->0.70*BiA0D+0.075*BiA1D+... k(1/T)=A/T,A=5.1e-8

HUMULE+OH->1.53*BiSQT+... k=1.97e-9

LIMONE+OH->0.35*BiA0D+0.20*BiA1D+0.0035*BiA2D+... k(T)=Aexp(-B/T),A=1.87e-11,B=-435

NO3 reactions:

APINEN+NO3->0.8*BiBmP+... k=1e-22

BPINEN+NO3->1.14*BiBmP+0.49*BiBIN+... k=2.51e-12

OCIMEN+NO3->1.74*BiA0D+0.087*BiA1D+0.087*BiA2D+... k(1/T)=A/T,A=4.30e-9

LIMONE+NO3->1.74*BiA0D+0.087*BiA1D+0.087*BiA2D+... k(T)=Aexp(-B/T),A=1.28e-12,B=-490

HUMULE+NO3->1.53*BiSQT+... k=1.90e-10

O3 reactions:

APINEN+O3->0.18*BiA0D+0.16*BiA1D+0.05*BiA2D+... k(T)=Aexp(-B/T),A=9.57e-16,B=785

BPINEN+O3->0.09*BiA0D+0.13*BiA1D+0.04*BiA2D+... k=1.5e-17

OCIMEN+O3->0.50*BiA0D+0.0.055*BiA1D+... k(1/T)=A/T,A=7.5e-14

LIMONE+O3->0.09*BiA0D+0.10*BiA1D+… k=2e-16

HUMULE+O3->1.53*BiSQT+… k=1.16e-13