Atmospheric
Chemistry
and Physics

Supplement of

Simulation of the effects of low-volatility organic compounds on aerosol number concentrations in Europe

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22 **Table S1:** Boundary and initial conditions of the gases, PM, and number concentration of the

23 simulation.

Gas (ppb)	Boundary conditions				Initial conditions
	WEST	EAST	SOUTH	NORTH	
Sulfur dioxide (SO_2)	1×10^{-2}	1×10^{-2}	1×10^{-2}	1×10^{-2}	1×10^{-2}
Ozone (O_3)	35	35	35	35	35
Nitric acid (HNO_3)	0.1	0.1	0.1	0.1	0.1
Formaldehyde (FORM)	5×10^{-2}	5×10^{-2}	5×10^{-2}	5×10^{-2}	5×10^{-2}
Ammonia (NH_3)	5×10^{-2}	5×10^{-2}	5×10^{-2}	5×10^{-2}	5×10^{-2}
Ethene (ETH)	5×10^{-3}	5×10^{-3}	5×10^{-3}	5×10^{-3}	5×10^{-3}
Carbon monoxide (CO)	50	50	50	50	50
Peroxynitric acid (HNO_4)	1×10^{-6}	1×10^{-6}	1×10^{-6}	1×10^{-6}	1×10^{-6}
Aerosol ($\mu g\ m^{-3}$)					
Dust (2.5 μm-10 μm)	1×10^{-9}	1×10^{-9}	1×10^{-9}	1×10^{-9}	1×10^{-9}
Sulfate (40 nm - 2.5 μm)	1×10^{-9}	1×10^{-9}	1×10^{-9}	1×10^{-9}	1×10^{-9}
SOA (40 nm - 2.5 μm)	6.6×10^{-7}	6.6×10^{-7}	6.6×10^{-7}	6.6×10^{-7}	6.6×10^{-7}
Number conc. (cm^{-3})	50	50	50	50	50

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33 **Table S2:** Description of atmospheric measurement sites in Europe used in this work.

Station	Name	Country	Longitude	Latitude
ANB	Annaberg-Buchholz	Germany	50.5717	12.9989
ASP	Aspvreten	Sweden	58.8000	17.3833
BRK	Birkenes II	Norway	58.3885	8.2520
CBW	Cabauw Zijdeweg	Netherlands	51.9703	4.9264
DSN	Dresden-Nord	Germany	51.0650	13.7414
DSW	Dresden-Winckelmannstrasse	Germany	51.0361	13.7306
FNK	Finokalia	Greece	35.3167	25.6667
GDN	Giordan Lighthouse	Malta	36.0722	14.2184
HOH	Hohenpeissenberg	Germany	47.8015	11.0096
HYY	Hyytiala	Finland	61.8500	24.2833
ISP	Ispra	Italy	45.8000	8.6333
KPU	K-puszta	Hungary	46.9667	19.5833
KST	Kosetice (NOAK)	Czech Republic	49.5734	15.0803
MLP	Melpitz	Germany	51.5301	12.9339
MNT	Montseny	Spain	41.7667	2.3500
PRG	Prague-Suchdol	Czech Republic	50.1264	14.3846
USM	Usti n.L.-mesto	Czech Republic	50.6611	14.0403
VAV	Vavihill	Sweden	56.0167	13.1500
VRR	Varrio	Finland	67.7667	29.5833
VSM	TMNT09 Vielsalm	Belgium	50.3040	6.0013
WLD	Waldhof	Germany	52.8022	10.7594
ZUG	Zugspitze-Schneefernerhaus	Germany	47.4165	10.9796
NEO	Costa Navarino	Greece	36.9932	21.6572
PAT	Patra-ICE-HT	Greece	38.2980	21.8092
SPC	San Pietro Capofiume	Italy	44.6553	11.6236
THE	Thessaloniki	Greece	40.6166	23.0333

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Table S3a: AMS PM$_1$ composition atmospheric measurement sites.

Station	Name	Country	Longitude	Latitude	Altitude (m)
FIN	Finokalia	Greece	35.3167	25.6667	250
PAT	Patra	Greece	38.2980	21.8092	85
BOL	Bologna	Italy	44.4833	11.3333	0
SPC	San Pietro Capofiume	Italy	44.6553	11.6236	11

Table S3b: Filter-based PM$_{2.5}$ composition measurements sites.

Station	Name	Country	Longitude	Latitude	Altitude (m)
CH02	Payerne	Switzerland	46.8131	6.9447	489
DE44	Melpitz	Germany	51.5301	12.9339	86
ES1778	Montseny	Spain	41.7667	2.3500	700
IT04	Ispra	Italy	45.8000	8.6333	209
PL05	Diabla Gora	Poland	54.1500	22.0667	157
SI08	Iskrba	Slovenia	45.5667	14.8667	520

50   **Table S4:** Prediction skill metrics of PMCAMx-UF for the base case against 3-min PM$_1$ measurements

51   during the PEGASOS Zeppelin flights.

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Species	Mean Observed Zeppelin (μg m^{-3})	Mean Predicted (μg m^{-3})	NMB (%)	NME (%)	Within Factor of 2 (%)
OA	4.60	4.40	-4	40	69
Sulfate	1.78	2.76	55	68	62
Ammonium	0.89	1.34	51	71	57
Nitrate	0.71	1.06	48	130	28

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Table S5: Prediction skill metrics of PMCAMx-UF for the simulation without ELVOCs against daily PM_1 OA measurements.

Station	Mean Predicted ($\mu g\ m^{-3}$)	Mean Observed ($\mu g\ m^{-3}$)	NMB (%)	NME (%)	Factor of 2 (%)
FIN	2.98	2.12	40	44	87
PAT	2.45	3.80	-35	35	90
BOL	4.29	5.68	-24	35	74
SPC	4.32	3.98	9	40	83
ALL	3.56	3.79	-6	38	83

Table S6: Prediction skill metrics of PMCAMx-UF for the simulation without ELVOCs against daily $PM_{2.5}$ OA measurements.

Name	Station	Country	Mean Observed ($\mu g\ m^{-3}$)	Mean Predicted ($\mu g\ m^{-3}$)	NMB (%)	NME (%)	Factor of 2 (%)
CH02	Payerne	Switzerland	2.54	2.02	-21	70	48
DE44	Melpitz	Germany	2.52	4.25	69	85	66
ES1778	Montseny	Spain	4.52	6.35	40	88	67
IT04	Ispra	Italy	5.13	5.74	12	48	68
PL05	Diabla Gora	Poland	3.64	3.81	5	40	84
SI08	Iskrba	Slovenia	5.98	5.15	-14	34	80
ALL			**4.06**	**4.55**	**15**	**61**	**69**

67   **Table S7:** Prediction skill metrics of PMCAMx-UF for the case without IVOCs against daily

68   ground measurements of particle number concentration above 10 nm (N_{10}) and 100 nm (N_{100})

69   during 5 June – 8 July 2012.

Station	Mean Observed	Mean Predicted	NMB	NME	Mean Observed	Mean Predicted	NMB	NME
	(cm^{-3})	(cm^{-3})	(%)	(%)	(cm^{-3})	(cm^{-3})	(%)	(%)
	N_{10}				N_{100}			
ANB	8057	6763	-16	37	1518	944	-38	46
ASP	2130	5310	149	149	552	748	36	57
BRK	1878	3158	68	89	607	403	-34	64
CBW	13101	10223	-22	29	1627	1448	-11	16
DSN	10591	6727	-36	39	1976	1144	-42	45
DSW	7706	6364	-17	38	1426	1123	-21	34
FNK	3962	5561	40	42	1760	2275	29	35
GDN	5712	6805	19	33	2492	2695	8	28
HOH	3438	3116	-9	40	1011	630	-38	40
HYY	2207	2488	13	29	677	566	-16	28
ISP	6232	6636	6	45	1775	1227	-31	39
KPU	5269	6069	15	45	1543	1797	16	26
KST	3596	5047	40	51	1123	1100	-2	25
MLP	5583	6223	11	43	1214	1064	-12	28
MNT	6455	8736	35	50	1492	1680	13	44
PRG	7272	7586	4	46	1177	1224	4	27
USM	15171	8764	-42	51	1657	1050	-37	40
VAV	3250	8496	161	161	766	922	20	49
VRR	1107	1107	0	51	324	158	-51	63
VSM	2903	7504	158	158	704	729	3	32
WLD	4956	8079	63	69	1116	993	-11	21
ZUG	1237	2450	98	114	555	497	-11	36
NEO	2864	5179	81	83	1489	1930	30	41
PAT	4705	5305	13	47	1747	1754	0	23
SPC	8301	7451	-10	35	1702	2020	19	35
THE	3894	8830	127	127	1387	2347	69	72
ALL	**4820**	**6125**	**27**	**65**	**1160**	**1240**	**5**	**43**

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Table S8: Prediction skill metrics of PMCAMx-UF for the simulation without IVOCs against daily PM$_1$ OA measurements.

Station	Mean Predicted (μg m^{-3})	Mean Observed (μg m^{-3})	NMB (%)	NME (%)	Factor of 2 (%)
FIN	2.44	2.12	15	26	93
PAT	2.25	3.80	-41	41	80
BOL	3.88	5.68	-32	36	78
SPC	3.80	3.98	-5	34	93
ALL	3.12	3.79	-18	35	87

Table S9: Prediction skill metrics of PMCAMx-UF for the simulation without IVOCs against daily PM$_{2.5}$ OA measurements.

| Name	Station	Country	Mean Observed (μg m^{-3})	Mean Predicted (μg m^{-3})	NMB (%)	NME (%)	Factor of 2 (%)
CH02	Payerne	Switzerland	2.54	2.08	-18	51	72
DE44	Melpitz	Germany	2.52	3.70	47	65	69
ES1778	Montseny	Spain	4.52	4.31	-5	61	67
IT04	Ispra	Italy	5.13	3.50	-32	45	65
PL05	Diabla Gora	Poland	3.64	3.56	-2	38	87
SI08	Iskrba	Slovenia	5.98	3.78	-37	37	80
ALL			**4.06**	**3.49**	**-8**	**50**	**73**

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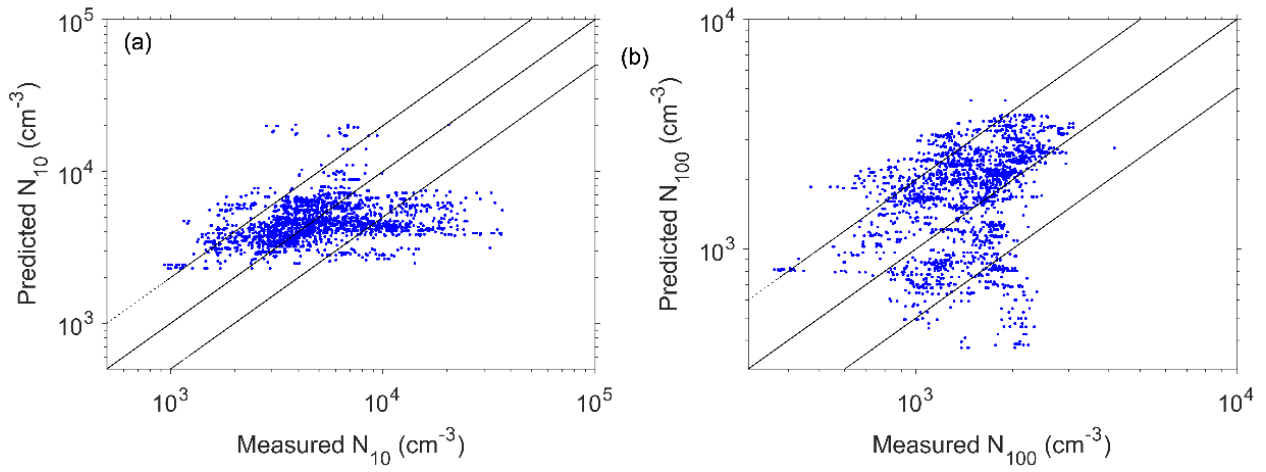
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90 **Figure S1:** Comparison of predicted (base case) versus observed (Zeppelin) 3-min particle number
91 concentrations (in cm^{-3}) for (a) N_{10} and (b) N_{100} of 25 flights over the Po Valley during the
92 PEGASOS campaign. There are approximately 2000 measurements included in the dataset. Also
93 shown the 1:1, 2:1 and 1:2 lines.

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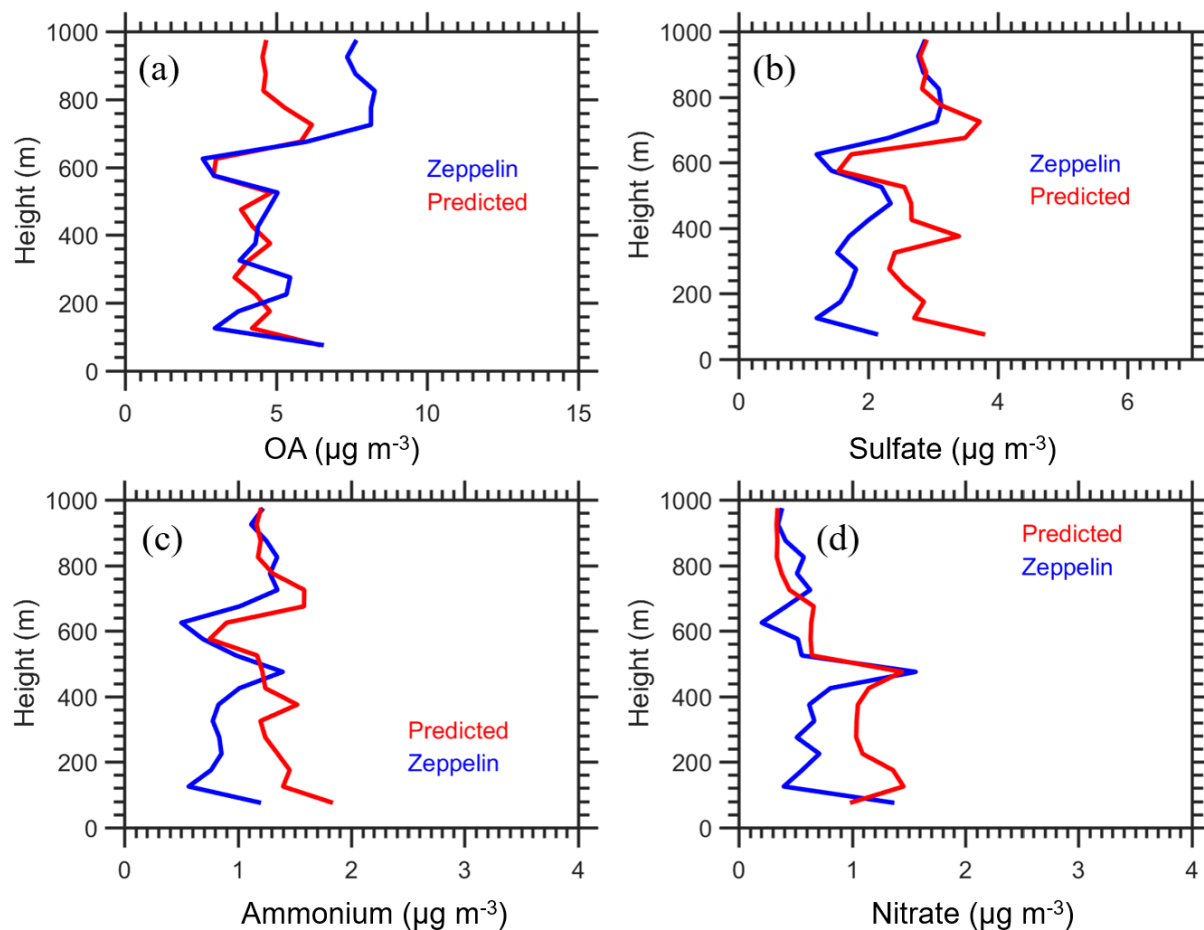
Figure S2: Comparison of predicted PMCAMx-UF (red lines) vs. observed (blue lines) vertical profiles of averaged PM_1 mass concentrations for (a) OA, (b) sulfate, (c) ammonium, and (d) nitrate (in $\mu g\ m^{-3}$) for 9 flights over the Po Valley during the PEGASOS campaign.
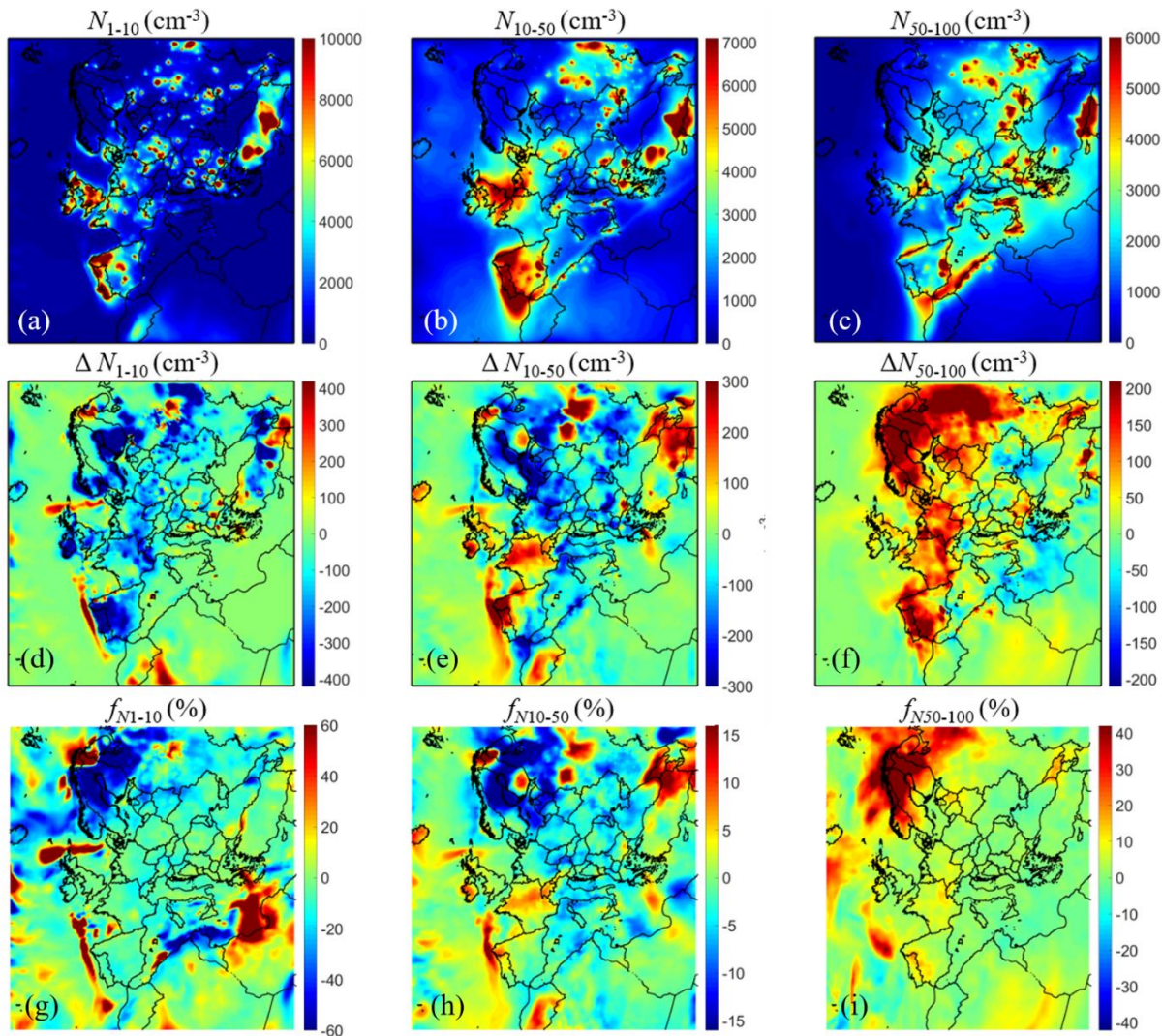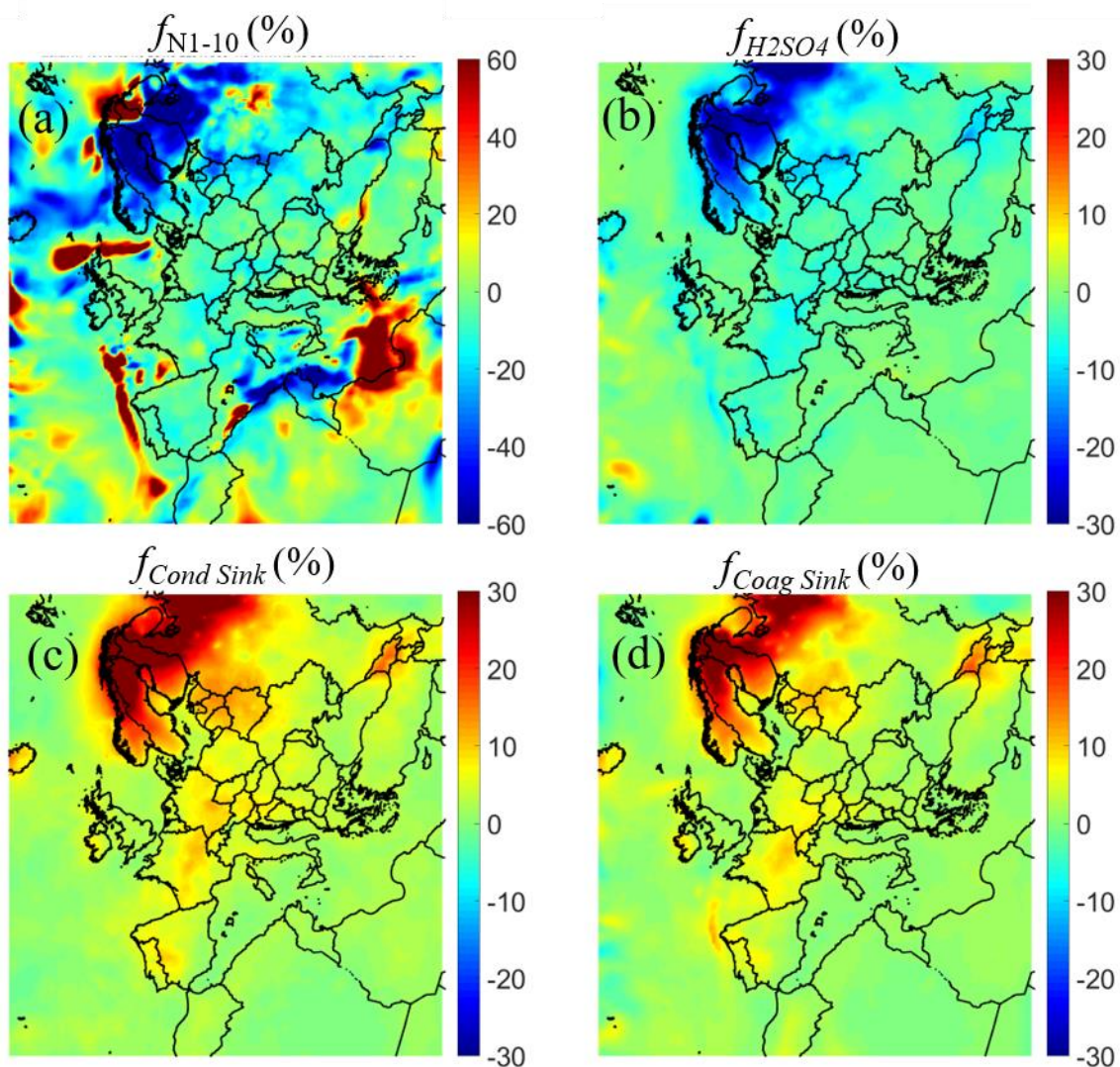
Figure S3: Average ground level number concentrations (in cm^{-3}) (a-b-c), increase of number concentration (in cm^{-3}) (d-e-f) and fractional increase (f_{Nx}) of number concentration (g-h-i) due to the condensation of ELVOCs during 5 June – 8 July 2012 for: (a-d-g) particles between 0.8 nm and 10 nm (N_{1-10}); (b-e-h) particles between 10 nm and 50 nm (N_{10-50}) and (c-f-i) particles between 50 nm and 100 nm (N_{50-100}). Different scales are used.
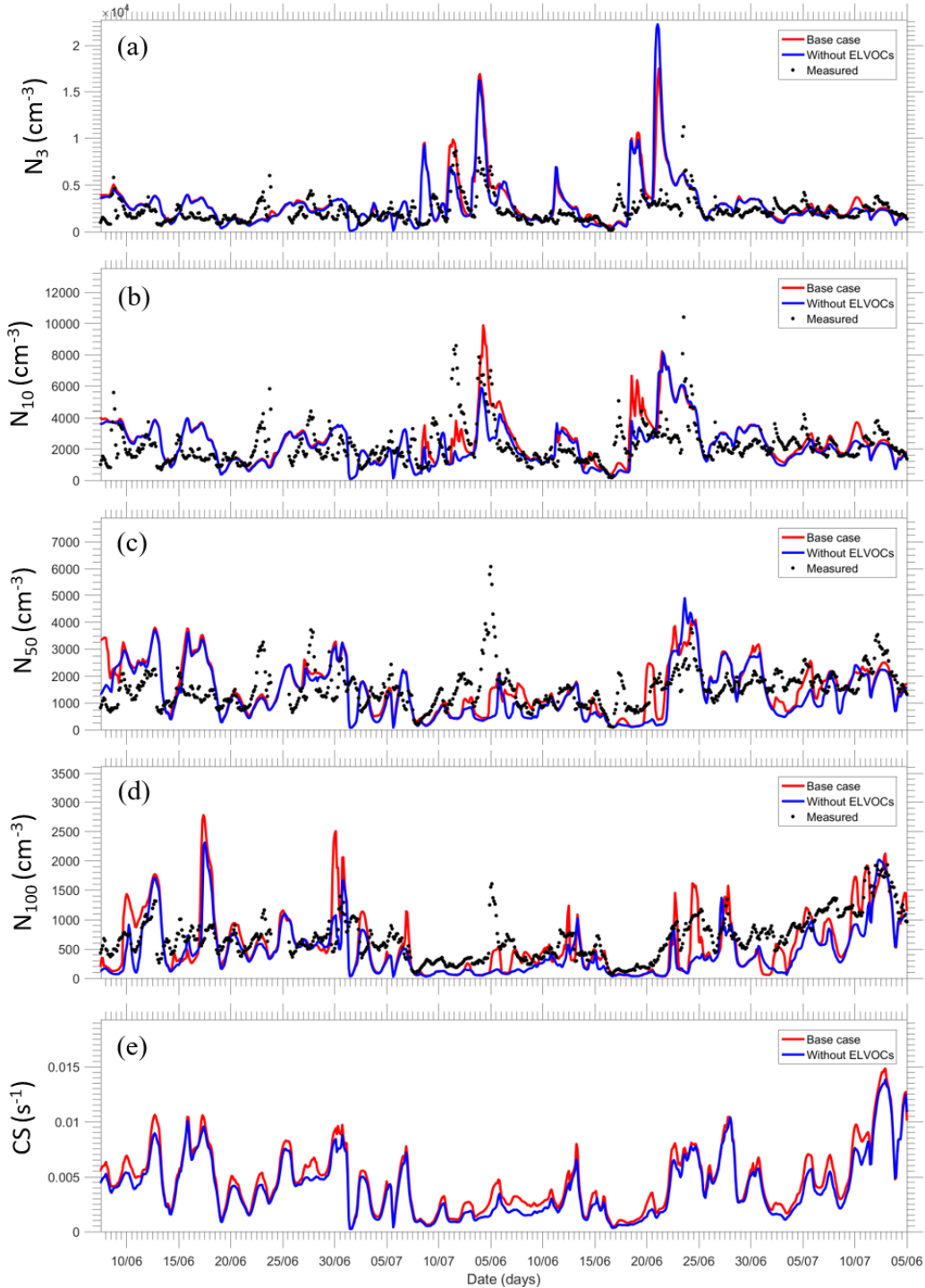
Figure S4: Average ground level fractional increase (*fNx*) due to the condensation of ELVOCs for: (a) number concentration particles between 0.8 nm and 10 nm (*fN1-10*); (b) sulfuric acid (gas phase); (c) condensation sink (*fCondSink*); and (d) coagulation sink (*fCoagSink*). Different scales are used.
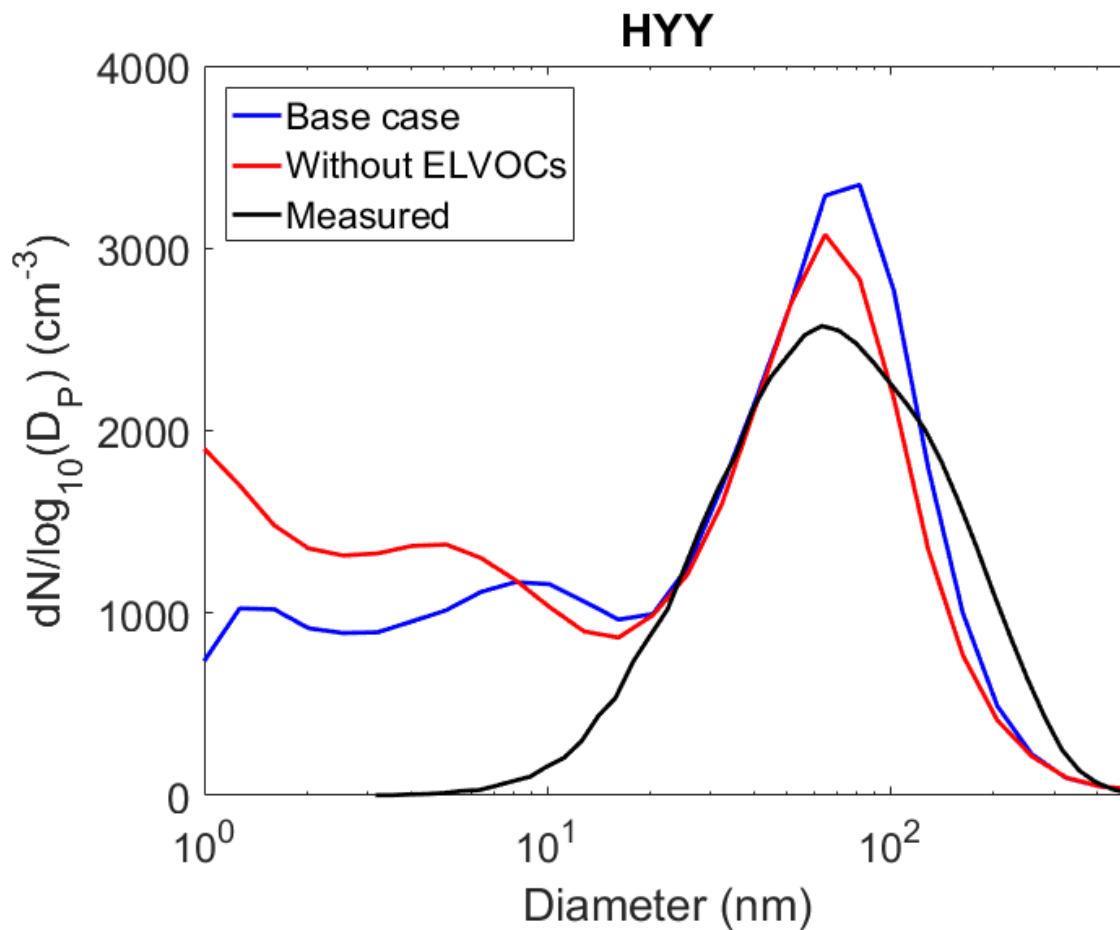
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Figure S5: Time series of particle number concentrations (in cm^{-3}) for (a) N_3, (b) N_{10}, (c) N_{50}, (d) N_{100} and condensation sink (in sec^{-1}) in Hyytiala during 5 June – 8 July 2012 with red line the predictions of PMCAMx-UF for the base case, blue lines the prediction of PMCAMx-UF for the case without ELVOCs and the black dots are the measurements.

Figure S6: Average number size distribution in Hyytiala during 5 June – 8 July 2012. The red line is the prediction of PMCAMx-UF for the base case simulation, the blue line is the prediction of PMCAMx-UF for the case without ELVOCs and the black line is the measured distribution (the smallest particles were not included in these measurements).