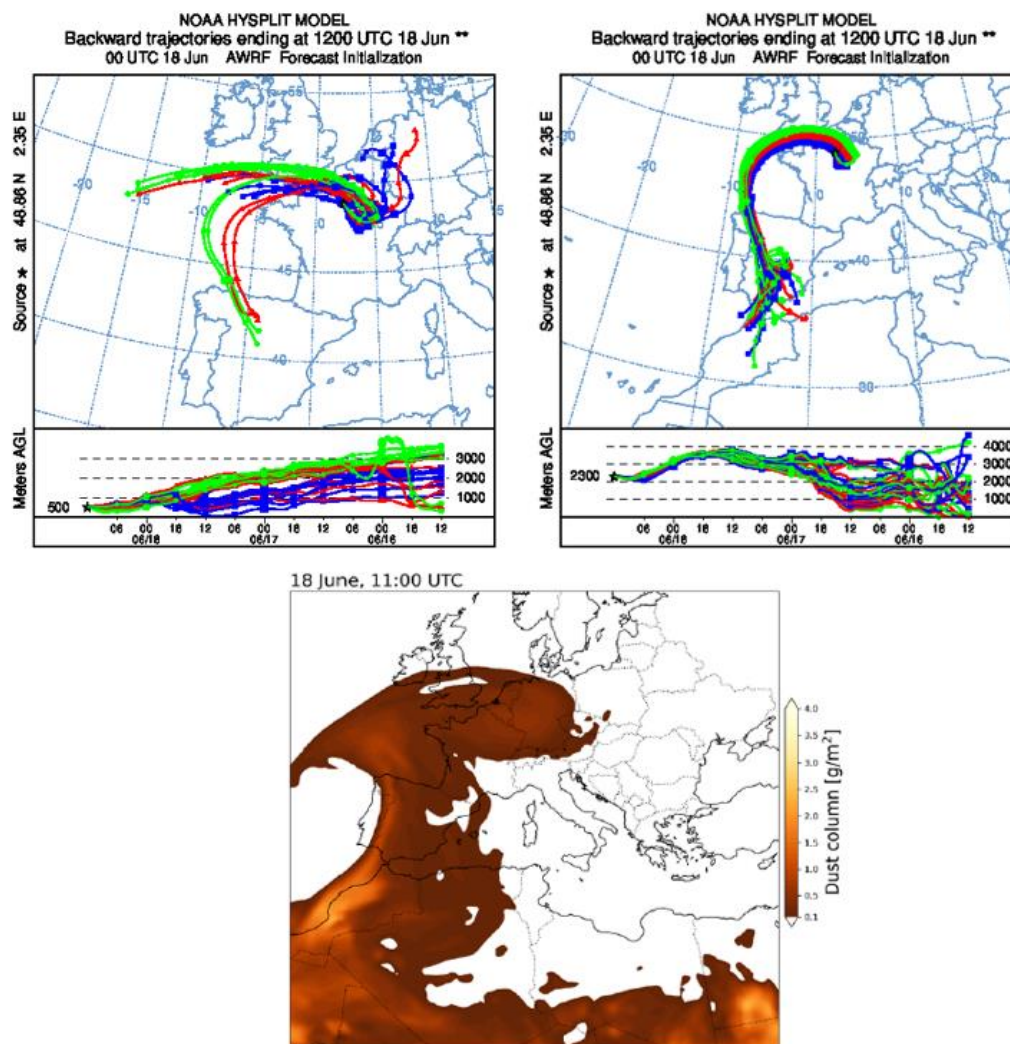
Supplementary material to "Modelling of atmospheric variability of gas and aerosols during the ACROSS campaign 2022 in the greater Paris area: evaluation of the meteorology, dynamics and chemistry"

5   **Figure S1 (Top) 3–day HYSPLIT backward trajectory simulations from (Siour and Di Antonio, 2023) for the 18 June 2022 starting in the center of Paris at an altitude of 500m (left) and 2000 m (right). (Bottom) Simulated dust columnar concentrations on the 18 June 2022 at 11:00 UTC. The dust plume reached northern Europe and the Paris area during the day.**

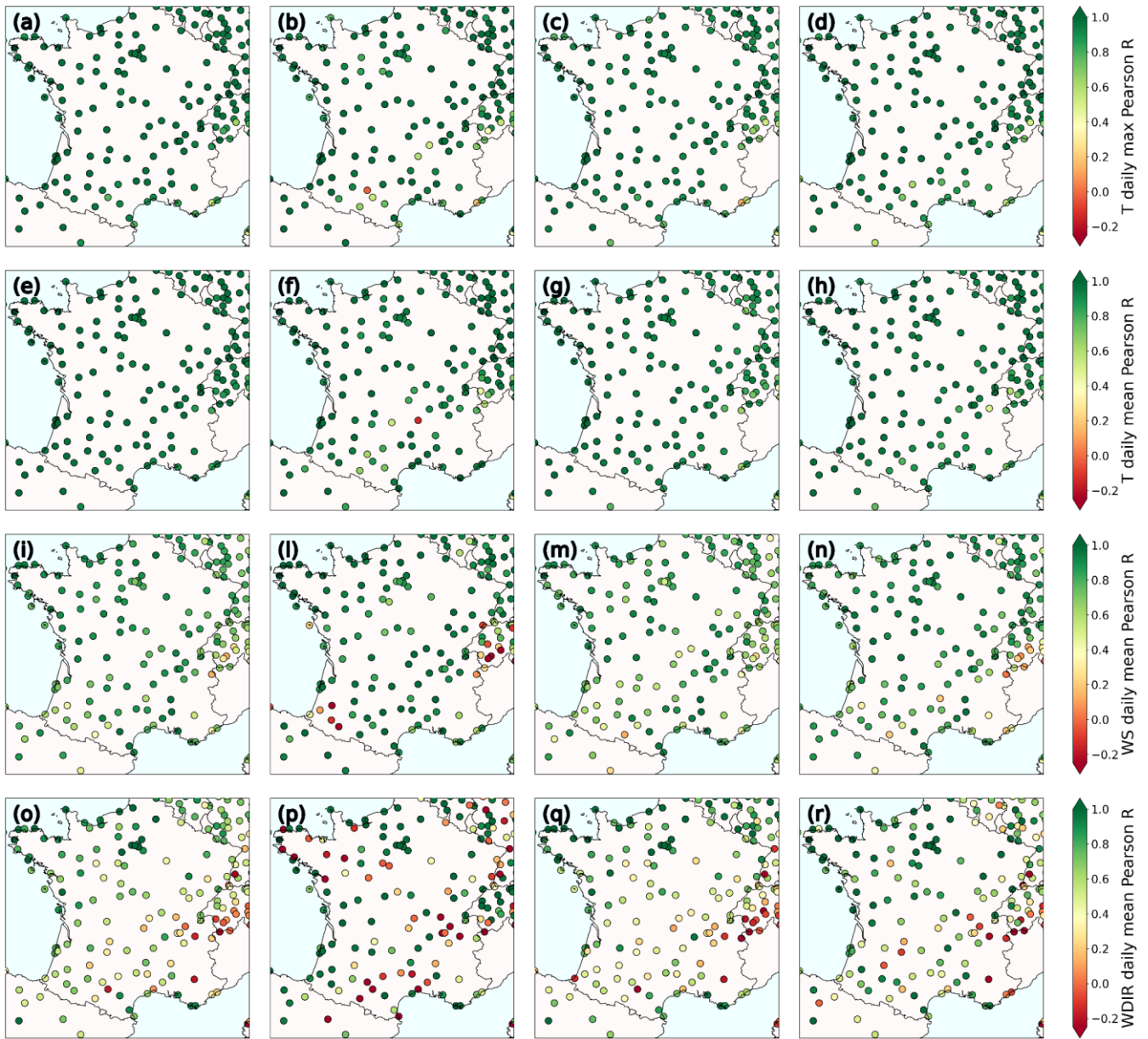



Figure S2: Daily Pearson correlation coefficient between WRF–CHIMERE model output and observations of the MIDAS database respectively for the full period (left column), the first heatwave (middle left column), the clean period (middle right column) and the second heatwave (right column); (a)–(d) for the temperature daily max, (e)–(h) temperature daily mean, (i)–(n) wind speed daily mean and (o)–(r) wind speed daily mean.

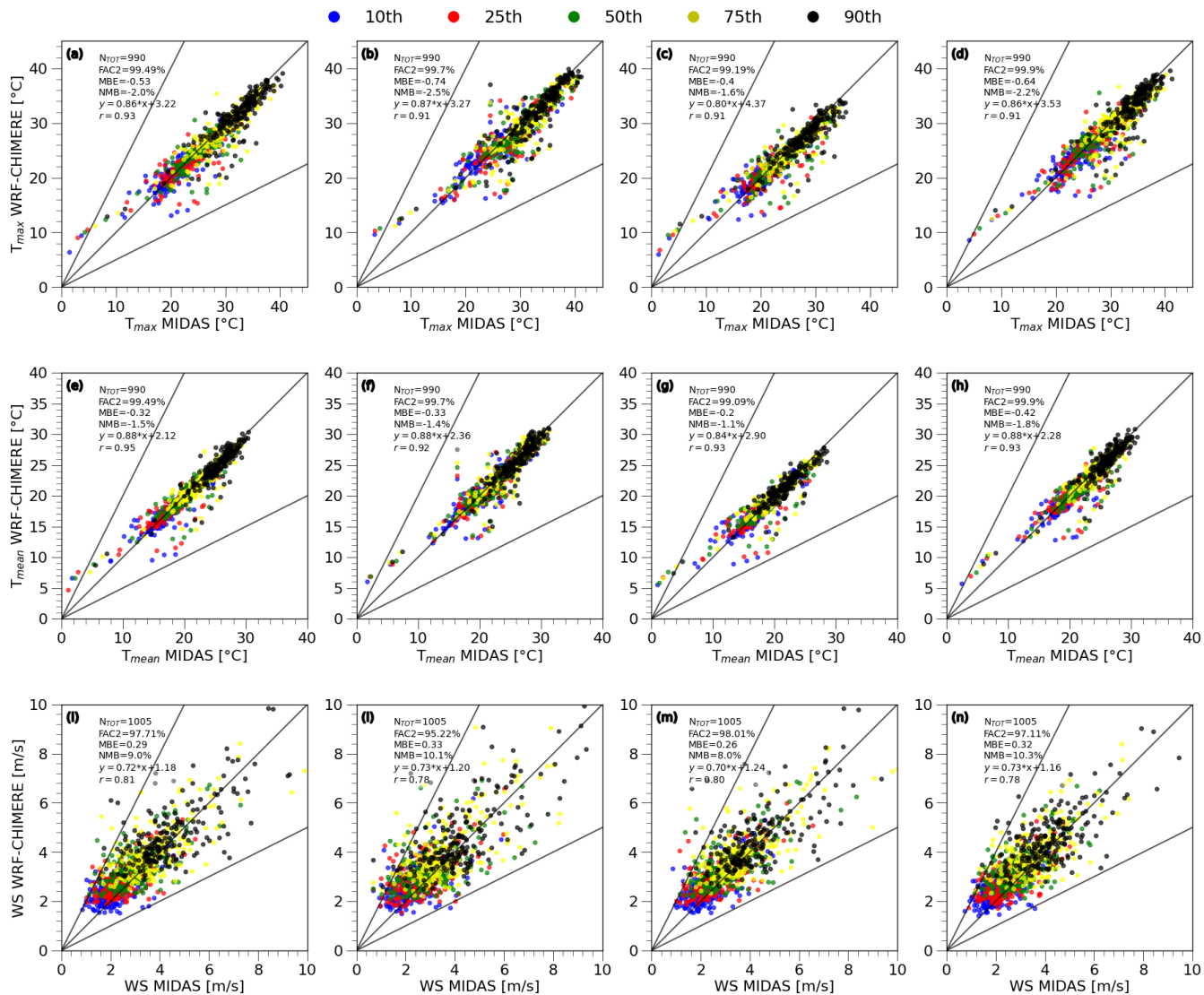



Figure S3: Percentile analysis of the WRF–CHIMERE simulated meteorological parameters compared to the MIDAS database observations, respectively for the full period (left column), the first heatwave (middle left column), the clean period (middle right column) and the second heatwave (right column) for the (a)–(d) temperature max, (e)–(h) temperature mean, (i)–(n) wind speed. Statistical metrics are calculated from data merged for all sites: NTOT number of observations, FAC2 fraction of points within a factor of 2 limit, MBE mean bias error, NMB normalized mean bias, linear fit equation, R correlation coefficient. The percentiles are calculated on the entire period of simulation and for each site available.

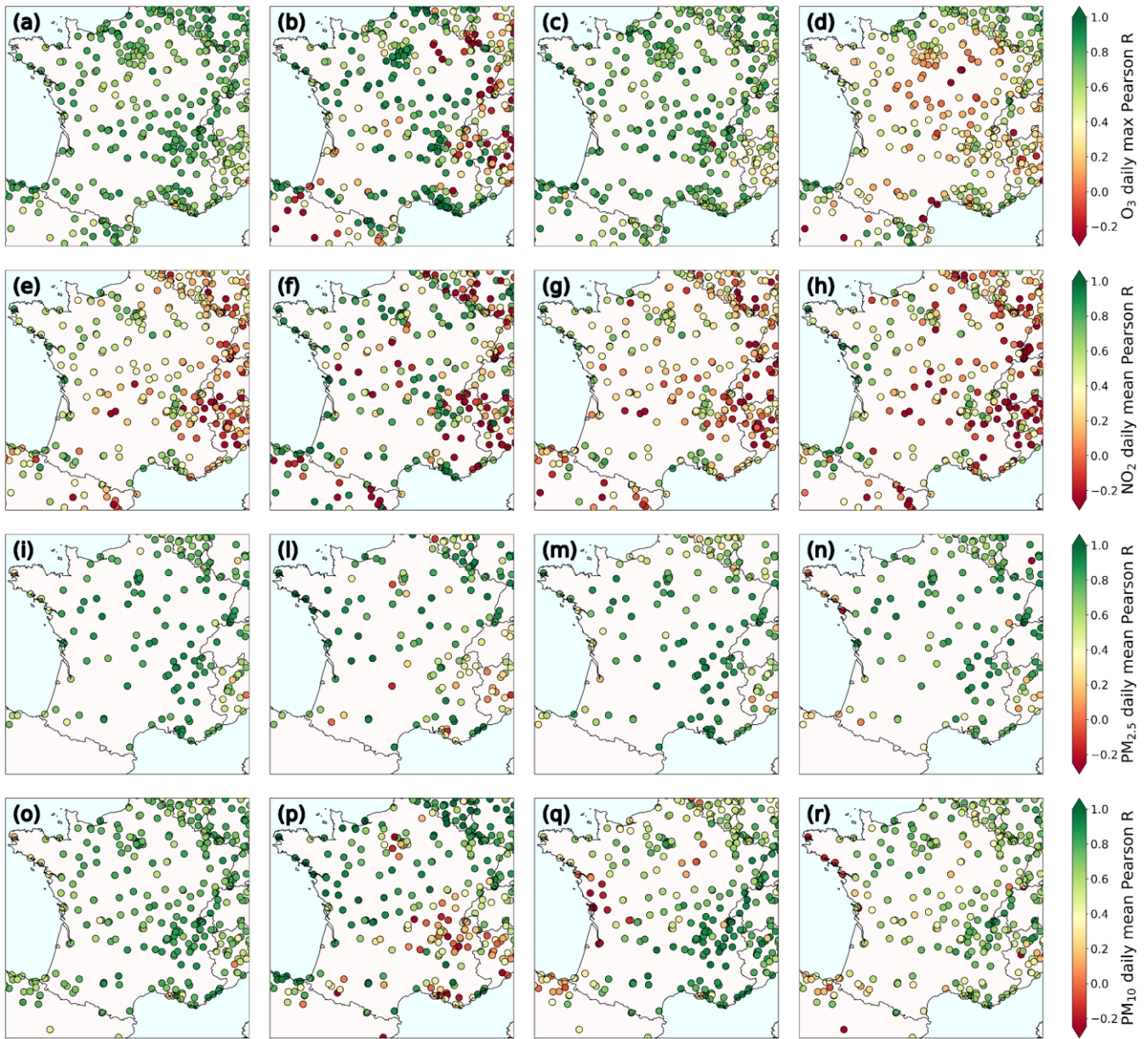



Figure S4: Daily Pearson correlation coefficients between WRF–CHIMERE output and EEA observations, respectively for the full period (left column), the first heatwave (middle left column), the clean period (middle right column) and the second heatwave (right column) for the (a)–(d) O3 daily max, (e)–(h) NO2 daily mean, (i)–(n) PM2.5 daily mean and (o)–(r) PM10 daily mean.

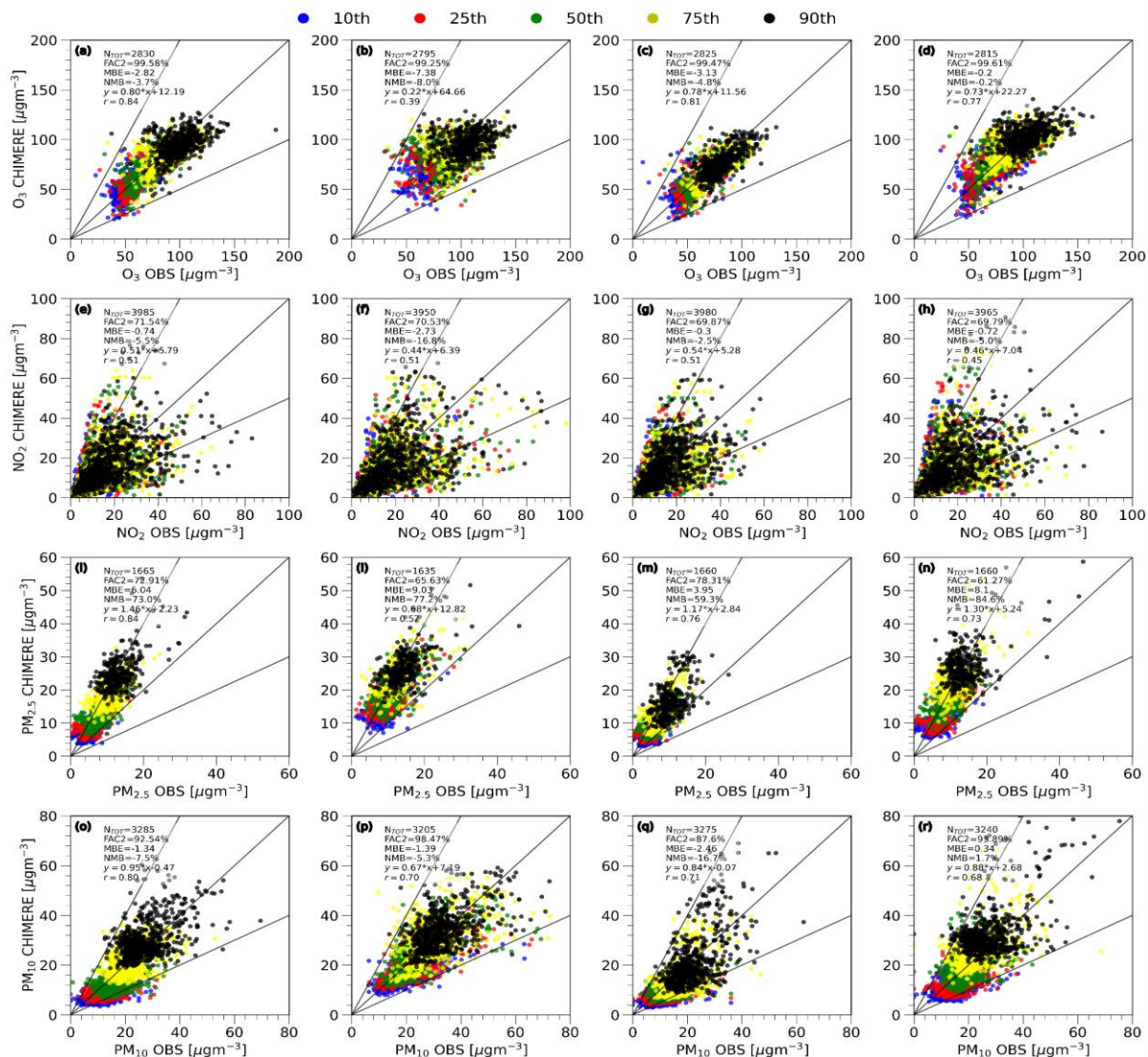



Figure S5: Percentile analysis of the WRF–CHIMERE simulated aerosol load and gaseous compounds compared to EEA observations, respectively for the full period (left column), the first heatwave (middle left column), the clean period (middle right column) and the second heatwave (right column) for the (a)–(d) O3, (e)–(h) NO2, (i)–(n) PM2.5, (o)–(r) PM10. Statistical metrics are calculated from data merged for all sites: NTOT number of observations, FAC2 fraction of points within a factor of 2 limit, MBE mean bias error, NMB normalized mean bias, linear fit equation, R correlation coefficient. Percentiles are calculated from the daily max values for O3, and from the daily means for PM10, NO2, PM2.5. The percentiles are calculated on the entire period of simulation and for each site available.

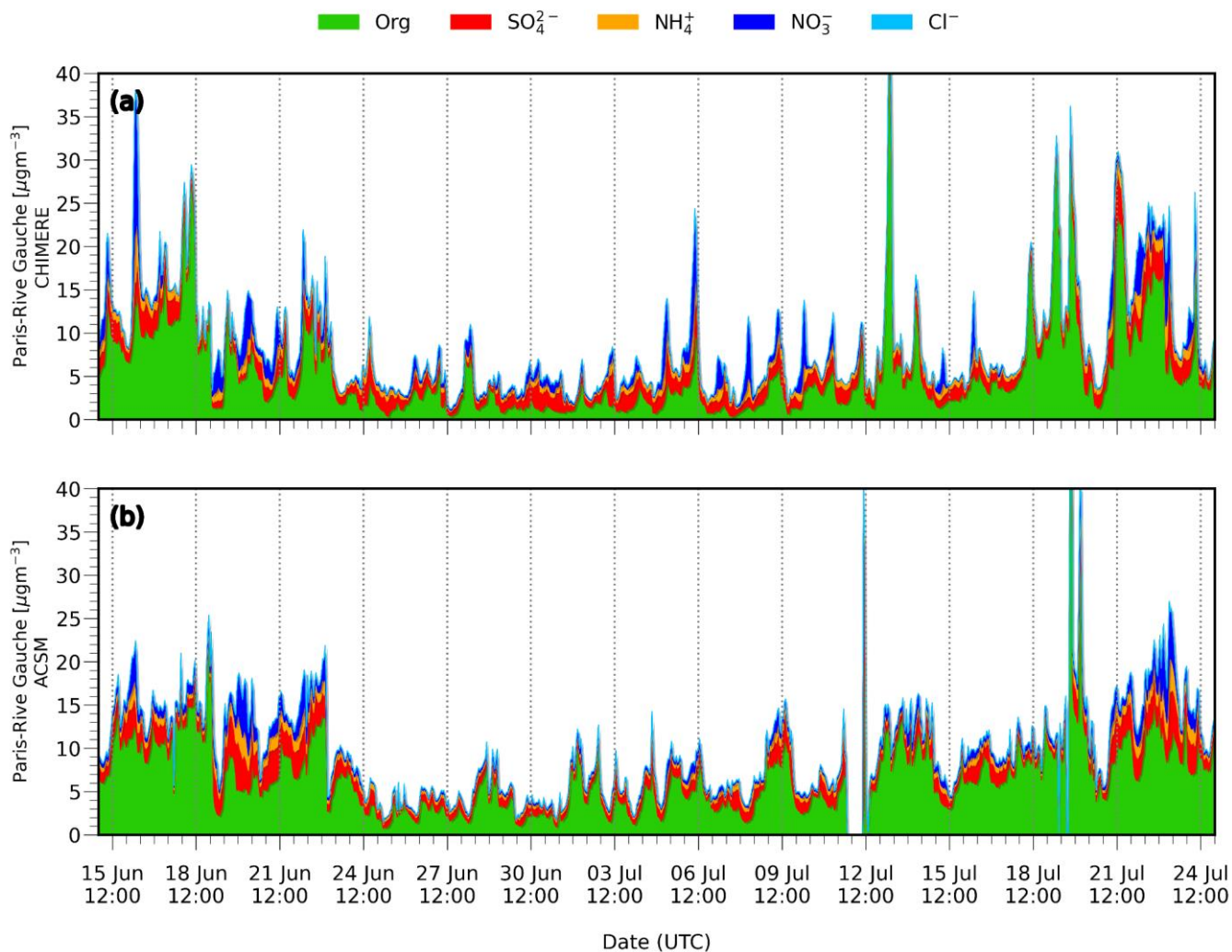



Figure S6: Time series of the chemical composition (organics, sulfate, nitrate, ammonium and chloride) simulated (a) and observed (b) at the Paris–Rive Gauche (PRG) urban background site.

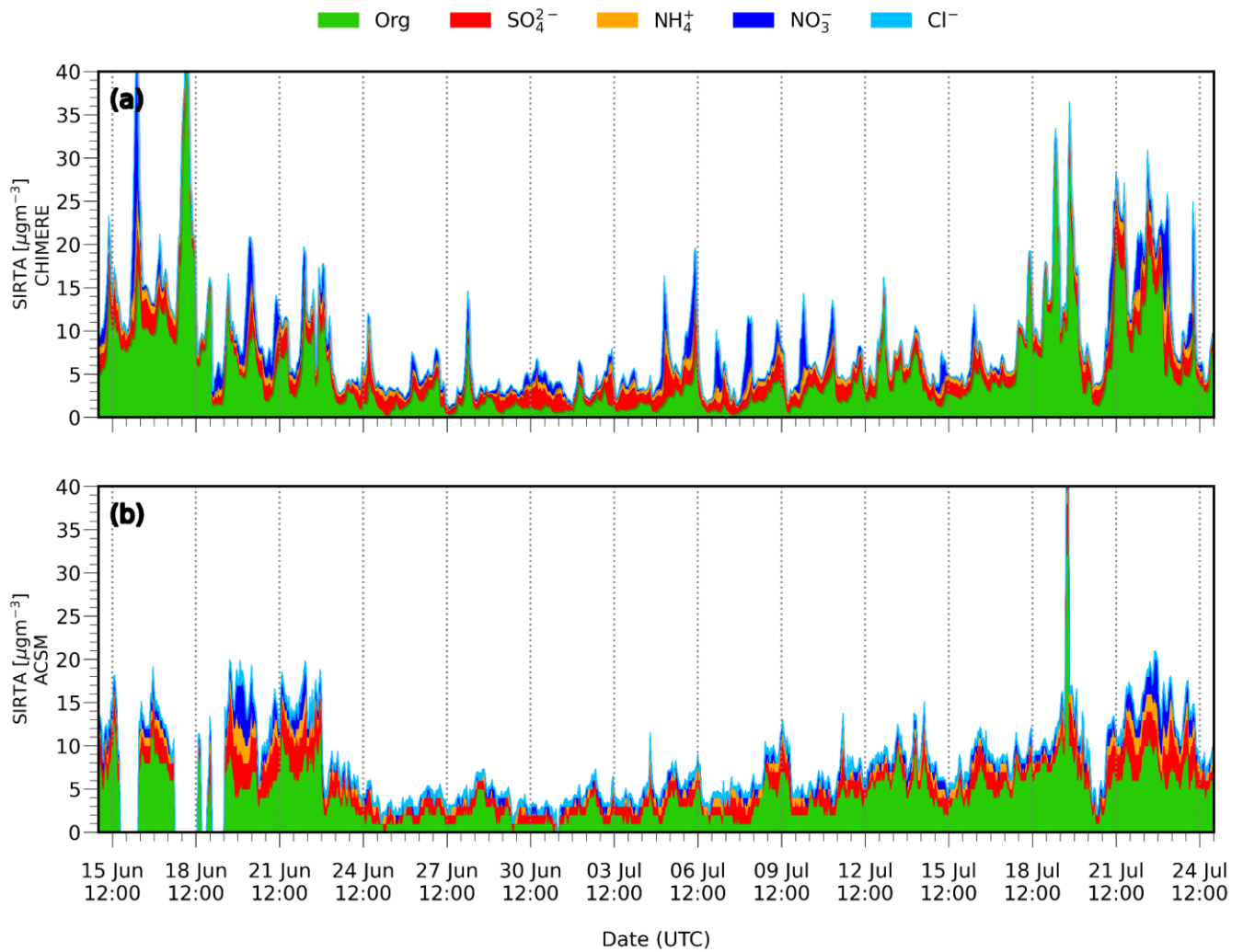



Figure S7: Time series of the chemical composition (organics, sulfate, nitrate, ammonium and chloride) simulated (a) and observed (b) at the SIRTA peri–urban site.

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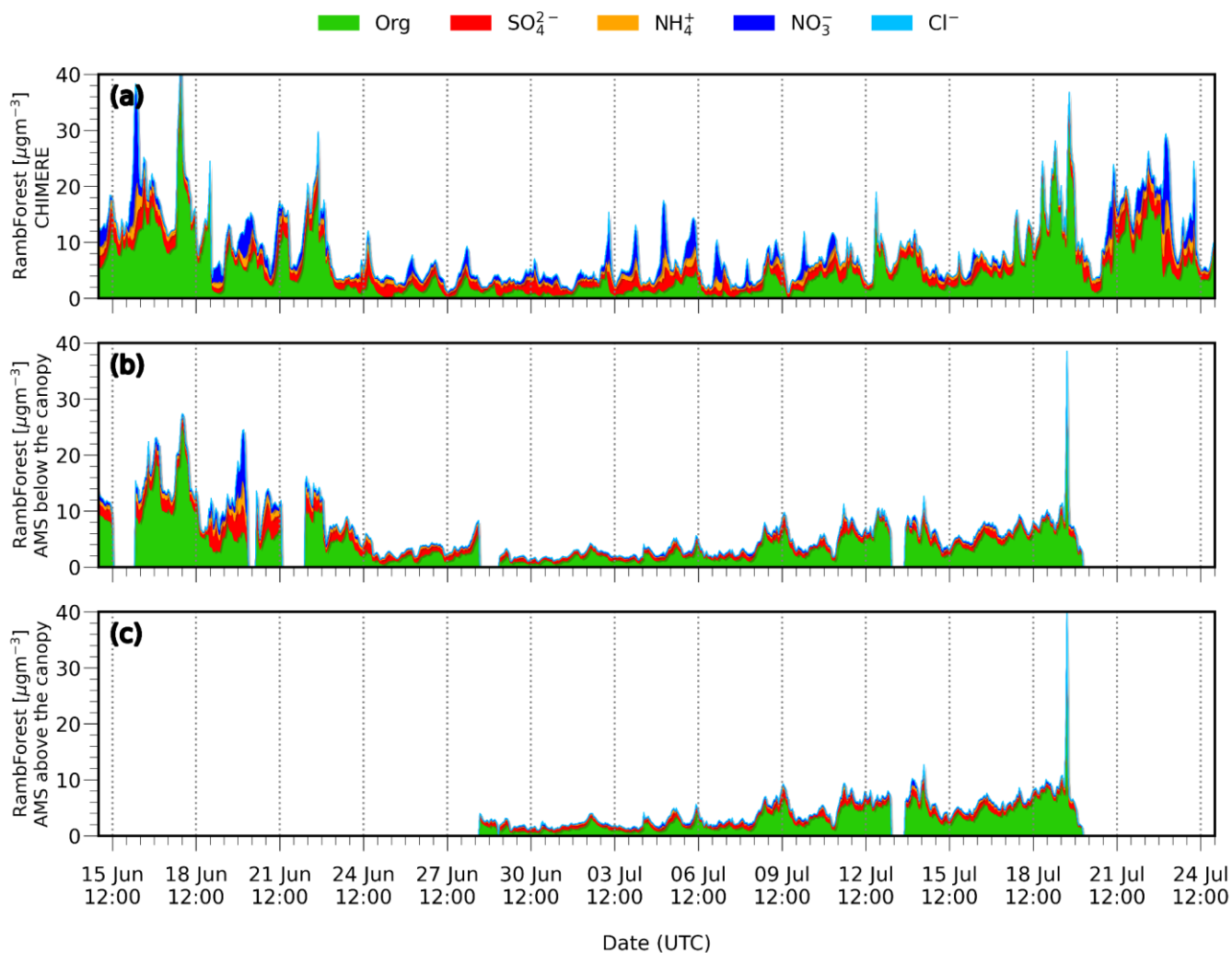
Figure S8: Time series of the chemical composition (organics, sulfate, nitrate, ammonium and chloride) simulated (a) and observed below the canopy (b) and above the canopy (c) at the Rambouillet forest (RambForest) site.

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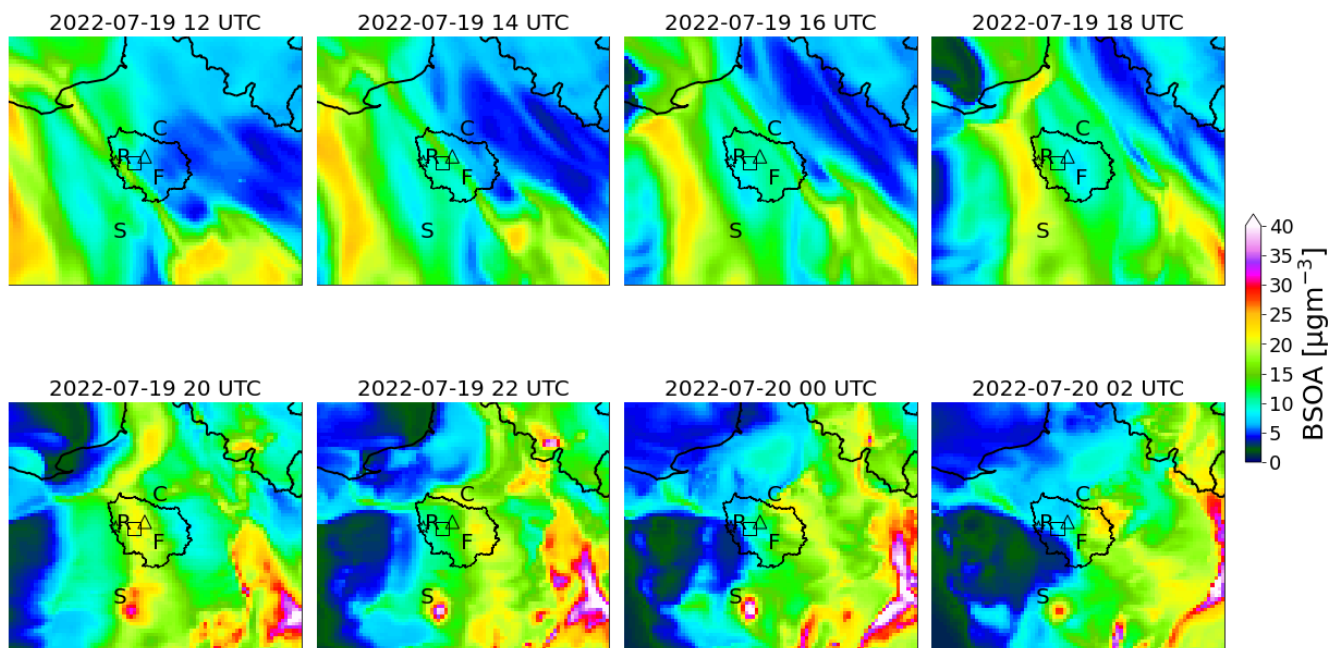
Figure S9: Simulated biogenic secondary organic aerosol (BSOA) mass concentrations for the 19 and 20 July 2022. "F" indicates the Fontainebleau forest, "R" the Rambouillet forest, "S" the Sologne forest and "C" the Chantilly forest. The star, the square and the triangle markers indicate respectively the RambForest, SIRTA and PRG sites. Please note that BSOA stems from BVOC compounds emitted by both fires and forests.

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Name	Longitude (° E)	Latitude (° N)	Features
Calais	1.84	50.94	Urban
Creil	2.47	49.25	Urban
Metz	6.22	49.11	Urban
Paris Les Halles	2.34	48.86	Urban
Strasbourg	7.76	48.57	Urban
Poitiers	0.34	46.58	Urban
Lyon	4.85	45.75	Urban
Toulouse	1.43	43.62	Urban
Marseille	5.39	43.30	Urban

Table S1: GEOD'AIR sites available to validate the aerosol chemical composition.

	Full period (15 June– 25 July)				First heatwave (15 June–19 June)				Clean period (20 June–11 July)				Second heatwave (12 July–25 July)			
	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %
Ammonium	943	0.52	0.06	8.2	120	0.39	0.11	12.8	524	0.40	0.10	16.5	299	0.71	–0.03	–3.9
Sulfate	942	0.25	–0.02	–1.2	120	–0.18	–0.21	–10.6	524	0.10	0.08	5.3	298	0.36	–0.11	–5.7
Nitrate	943	0.47	0.11	15.2	120	0.65	0.27	28.7	524	0.46	0.30	55.6	299	0.53	–0.29	–29.8
Organic	943	0.61	–1.39	–19.9	120	0.54	0.02	0.10	524	0.53	–1.78	–37.7	299	0.44	–1.26	–13.3
Chloride	943	0.14	–0.001	–1.7	120	0.56	–0.02	–45.2	524	–0.10	0.01	44.0	299	0.39	–0.02	–35.4
	OBS		MOD		OBS		MOD		OBS		MOD		OBS		MOD	
Ammonium	0.72		0.78		0.87		0.98		0.60		0.70		0.86		0.83	
Sulfate	1.66		1.64		2.9		1.79		1.42		1.50		1.93		1.82	
Nitrate	0.72		0.83		0.94		1.22		0.54		0.84		0.96		0.68	
Organic	6.97		5.58		10.60		10.61		4.71		2.93		9.46		8.20	
Chloride	0.04		0.04		0.04		0.02		0.03		0.05		0.06		0.04	

Table S2: Summary of the comparison of model output to observations for the PRG (urban) site from the ACSM; Statistical metrics are: NTOT, number of observations; R, correlation coefficient; MBE, mean bias error; NMB, normalized mean bias.

	Full period (15 June– 25 July)				First heatwave (15 June–19 June)				Clean period (20 June–11 July)				Second heatwave (12 July–25 July)			
	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %
Ammonium	904	0.50	0.01	0.7	68	0.002	–0.15	–13.7	524	0.35	0.10	17.9	412	0.73	–0.13	–14.4
Sulfate	906	0.37	–0.22	–12.0	68	–0.37	–0.63	–22.9	526	0.20	–0.11	–6.9	312	0.64	–0.32	–15.6
Nitrate	906	0.39	0.13	21.0	68	0.13	–0.24	–28	526	037	0.33	63.8	312	0.50	–0.12	–15.5
Organic	906	0.68	–0.16	–3.1	68	0.08	1.93	22.6	526	0.65	–0.90	–24.5	312	0.52	0.64	9.1
Chloride	888	0.11	0.003	7.9	68	–0.01	–0.01	–38.1	511	–0.49	0.01	30.5	309	0.71	–0.01	–17.3
	OBS		MOD		OBS		MOD		OBS		MOD		OBS		MOD	
Ammonium	0.75		0.75		1.07		092		0.60		0.71		0.93		0.80	
Sulfate	1.86		1.63		2.73		2.10		1.62		1.51		2.07		1.74	
Nitrate	0.62		0.75		0.87		0.63		0.51		0.84		0.76		0.64	
Organic	5.18		5.03		8.54		10.48		3.68		2.78		7.00		7.64	
Chloride	0.038		0.041		0.035		0.021		0.037		0.048		0.041		0.033	

85   **Table S3: As Table S2, but for the SIRTA (suburban) site**

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	Full period (15 June– 25 July)				First heatwave (15 June–19 June)				Clean period (20 June–11 July)				Second heatwave (12 July–25 July)			
	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %
Above the canopy																
Ammonium	506	0.07	0.46	251.8			–		319	0.16	0.57	396.0	187	0.36	0.26	106.5
Sulfate	506	0.01	0.67	95.9			–		319	0.01	0.81	130.7	187	0.31	0.43	51.3
Nitrate	506	0.21	0.52	325.4			–		319	0.52	0.84	632.7	187	0.17	−0.02	−6.9
Organic	506	0.62	0.7	21.3			–		319	0.57	−0.04	−1.7	187	0.41	1.99	36.7
Chloride	506	0.139	0.015	59.4			–		319	0.12	0.027	99.6	187	0.20	−0.005	−21.4
Below the canopy																
Ammonium	772	0.27	0.33	89.3	101	0.18	0.19	23.3	484	0.22	0.40	123.2	187	0.43	0.24	93.0
Sulfate	772	0.17	0.40	36.7	101	−0.12	−0.18	−8.8	484	0.11	0.51	51.4	187	0.38	0.44	53.3
Nitrate	772	0.29	0.48	148.1	101	0.25	0.64	105.5	484	0.32	0.64	214.4	187	0.45	−0.035	−15.3
Organic	772	0.77	0.45	9.7	101	0.76	1.22	11.9	484	0.76	−0.13	−4.5	187	0.43	1.52	26.0
Chloride	772	0.06	0.01	32.8	101	0.61	−0.021	67.6	484	−0.08	0.02	67.6	187	0.39	0.0	−1.4
	OBS		MOD		OBS		MOD		OBS		MOD		OBS		MOD	
Ammonium	0.18/0.38		0.64/0.71		0.83		1.02		0.14/0.33		0.71/0.73		0.25/0.26		0.51/0.61	
Sulfate	0.70/1.09		1.38/1.49		2.08		1.90		0.63/0.99		1.45/1.49		0.83/0.82		1.26/1.26	

Nitrate	0.16/0.32	0.69/0.80	0.61	1.25	0.13/0.30	0.97/0.94	0.21/0.23	0.19/0.19
Organic	3.34/4.59	4.05/5.04	10.35	11.58	2.13/2.90	2.09/2.77	5.40/5.87	7.39/7.40
Chloride	0.025/0.031	0.040/0.041	0.052	0.028	0.027/0.031	0.05/0.053	0.023/0.018	0.018/0.017

Table S4: As Table S2, but for the RambForest site using using AMS measurements. Average concentrations are reported for both above and below the canopy, respectively, divided by a slash sign.

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	Full period (15 June– 25 July)				First heatwave (15 June–19 June)				Clean period (20 June–11 July)				Second heatwave (12 July–25 July)			
	N_{TOT}	R	MBE $\mu g\ m^{-3}$	NMB %	N_{TOT}	R	MBE $\mu g\ m^{-3}$	NMB %	N_{TOT}	R	MBE $\mu g\ m^{-3}$	NMB %	N_{TOT}	R	MBE $\mu g\ m^{-3}$	NMB %
eBC	70	0.50	0.11	25	10	0.60	0.20	34	36	0.17	0.12	40	23	0.53	–0.001	–0.1
EC	70	0.41	0.11	25	10	0.62	0.18	29	36	–0.04	0.14	48	23	0.36	–0.002	–3.5
OM	71	0.73	–0.17	–3	10	0.53	2.2	27	37	0.50	–1.2	–31	23	0.58	0.5	7
	OBS		MOD		OBS		MOD		OBS		MOD		OBS		MOD	
eBC	0.45		0.56		0.60		0.80		0.31		0.43		0.59		0.59	
EC	0.45				0.62				0.29				0.61			
OM	5.8		5.6		8.2		10.3		4.0		2.76		7.6		8.1	

Table S5: Summary of the comparison of the black carbon concentrations for the PRG (urban) site averaged on the filter sampling times (daytime 6 – 20 UTC, night time 20 – 6 UTC). eBC has been corrected for the ACTRIS harmonisation factor (H*=2.45). OC has been converted to OM assuming an OM/OC ratio equal to 1.8. Statistical metrics are: NTOT number of observations, R correlation coefficient, MBE mean bias error, NMB normalized mean bias.

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	Full period (15 June– 25 July)				First heatwave (15 June–19 June)				Clean period (20 June–11 July)				Second heatwave (12 July–25 July)			
	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %	N_{TOT}	R	MBE µg m^{-3}	NMB %
eBC	36	0.28	0.1	64			–		17	0.36	0.13	130	19	0.13	0.07	36
EC	38	0.38	0.1	60			–		17	0.3	0.13	130	21	0.32	0.07	34
rBC	21	0.45	0.17	153			–		1	–	–	–	20	0.47	0.16	147
OM	40	0.82	0.18	4			–		19	0.70	−1.10	−29	21	0.70	1.27	19
	OBS	MOD			OBS	MOD			OBS	MOD			OBS	MOD		
eBC	0.15	0.25				–			0.10	0.22			0.20	0.27		
EC	0.16					–			0.10				0.21			
rBC	0.11					–			0.08				0.11			
OM	5.17	5.36				–			3.42	2.42			6.74	8.01		

Table S6: As for Table S5, but for the RambForest (forest) site.