Supplementary Information

Simulation of the chemical evolution of biomass burning organic aerosol

G. N. Theodoritsi[1,2] and S. N. Pandis[1,2,3]

[1]*Department of Chemical Engineering, University of Patras, Patras, Greece*

[2]*Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas (FORTH/ICE-HT), Patras, Greece*

[3]*Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, USA*

Table S1. POA and bbPOA emission rates (in tn d^{-1}) for each volatility bin during the simulated periods.

C^* at 298 K ($\mu g\ m^{-3}$)	10^{-2}	10^{-1}	10^{0}	10^{1}	10^{2}	10^{3}	10^{4}	10^{5}	10^{6}
1-29 May 2008 emission rate (tn d^{-1})									
fPOA	100	200	310	480	620	1000	1400	1700	2700
bbPOA (Base case)	530	0	260	260	530	260	800	1300	2100
bbPOA (Sensitivity test)	580	0	290	290	580	290	870	-	-
25 February – 22 March 2009 emission rate (tn d^{-1})									
fPOA	70	140	210	330	420	700	930	1200	1900
bbPOA (Base case)	2100	0	1000	1000	2100	1000	3100	5100	8200
bbPOA (Sensitivity test)	2300	0	1100	1100	2300	1100	3400	-	-

Table S2. Prediction skill metrics of PMCAMx-SR (base case) against AMS factor analysis in May 2008[a].

	Mean Observed ($\mu g\ m^{-3}$)	Mean Predicted ($\mu g\ m^{-3}$)	MB ($\mu g\ m^{-3}$)	MAGE ($\mu g\ m^{-3}$)	FBIAS	FERROR
			Cabauw			
OA	4.37	5.55	1.18	1.68	0.30	0.39
HOA	0.59	0.33	-0.27	0.31	-0.56	0.69
BBOA	0.43	0.42	-0.01	0.36	-0.18	0.53
OOA	3.34	4.80	1.46	1.64	0.42	0.46
			Finokalia			
OA	2.49	3.00	0.50	0.92	0.21	0.36
HOA	0.09	0.03	-0.06	0.07	-0.81	0.97
BBOA	-	0.03	-	-	-	-
OOA	2.41	2.94	0.54	0.92	0.23	0.37
			Melpitz			
OA	5.12	4.45	-0.68	1.32	-0.13	0.28
HOA	0.27	0.14	-0.13	0.17	-0.62	0.83
BBOA	-	0.12	-	-	-	-
OOA	4.86	4.19	-0.66	1.29	-0.14	0.29
			Mace Head			
OA	2.29	2.62	0.34	1.08	0.05	0.43
HOA	0.28	0.07	-0.21	0.21	-1.09	1.12
BBOA	0.39	0.04	-0.35	0.35	-1.66	1.66
OOA	1.61	2.51	0.89	1.12	0.34	0.50

[a]Number of datapoints; Cabauw: 623, Finokalia: 494, Melpitz: 155, Mace Head: 329

Table S3. Prediction skill metrics of PMCAMx-SR (sensitivity test) against AMS factor analysis in May 2008[a].

	Mean Observed ($\mu g\ m^{-3}$)	Mean Predicted ($\mu g\ m^{-3}$)	MB ($\mu g\ m^{-3}$)	MAGE ($\mu g\ m^{-3}$)	FBIAS	FERROR
Cabauw						
OA	4.37	5.23	0.86	1.49	0.25	0.36
HOA	0.59	0.33	-0.27	0.32	-0.57	0.71
BBOA	0.43	0.46	0.03	0.38	-0.14	0.54
OOA	3.34	4.44	1.10	1.35	0.35	0.41
Finokalia						
OA	2.45	2.72	0.22	0.79	0.12	0.33
HOA	0.09	0.03	-0.07	0.07	-0.83	0.99
BBOA	-	0.03	-	-	-	-
OOA	2.41	2.65	0.25	0.77	0.14	0.33
Melpitz						
OA	5.12	4.16	-0.96	1.38	-0.19	0.29
HOA	0.27	0.13	-0.13	0.17	-0.63	0.84
BBOA	-	0.13	-	-	-	-
OOA	4.86	3.89	-0.96	1.34	-0.21	0.31
Mace Head						
OA	2.29	2.49	0.20	0.99	0.01	0.42
HOA	0.28	0.07	-0.21	0.21	-1.11	1.13
BBOA	0.39	0.05	-0.34	0.34	-1.63	1.63
OOA	1.61	2.37	0.76	1.01	0.29	0.48

[a]Number of datapoints; Cabauw: 623, Finokalia: 494, Melpitz: 155, Mace Head: 329

Table S4. Prediction skill metrics of PMCAMx-SR (base case) against AMS factor analysis during 25 February – 23 March 2009[a].

	Mean Observed ($\mu g\ m^{-3}$)	Mean Predicted ($\mu g\ m^{-3}$)	MB ($\mu g\ m^{-3}$)	MAGE ($\mu g\ m^{-3}$)	FBIAS	FERROR
Cabauw						
OA	1.34	2.53	1.19	1.50	0.58	0.79
HOA	0.25	0.55	0.30	0.38	0.71	0.90
BBOA	0.13	1.05	0.93	0.94	1.35	1.40
OOA	0.96	0.93	-0.03	0.53	0.11	0.68
Helsinki						
OA	2.84	3.85	1.01	1.28	0.37	0.43
HOA	0.45	0.29	-0.16	0.25	-0.14	0.66
BBOA	0.40	1.67	1.27	1.27	1.19	1.19
OOA	1.99	1.89	-0.09	0.58	-0.02	0.37
Mace Head						
OA	0.95	0.64	-0.30	1.33	0.33	1.38
HOA	0.09	0.004	-0.09	0.09	-0.53	1.15
BBOA	0.34	0.01	-0.32	0.34	-0.42	1.24
OOA	0.61	0.63	0.02	0.99	0.38	1.37
Melpitz						
OA	1.62	1.23	-0.39	0.94	-0.26	0.71
HOA	0.15	0.09	-0.05	0.08	-0.31	0.68
BBOA	0.18	0.37	0.19	0.28	0.69	0.93
OOA	1.29	0.76	-0.52	0.85	-0.49	0.88
Hyytiala						
OA	1.45	2.36	0.92	1.12	0.55	0.66
HOA	0.05	0.14	0.09	0.09	0.83	0.93
BBOA	0.07	0.82	0.75	0.75	1.66	1.66
OOA	1.33	1.41	0.08	0.69	0.12	0.58
Barcelona						
OA	8.66	3.62	-5.04	5.31	-0.68	0.78
HOA	3.53	0.21	-3.32	3.32	-1.62	1.63
BBOA	0.69	1.09	0.41	0.72	0.46	0.80
OOA	4.45	2.32	-2.13	2.42	-0.51	0.69
Chilbolton						
OA	2.49	1.12	-1.39	1.54	-0.61	0.81
HOA	0.50	0.19	-0.32	0.33	-0.88	0.93
BBOA	0.49	0.24	-0.26	0.36	-0.72	1.07
OOA	1.49	0.69	-0.79	0.99	-0.55	0.87

[a]Number of datapoints; Cabauw: 418, Helsinki: 350, Mace Head: 206, Melpitz: 314, Hyytiala:426,Barcelona:485,Chilbolton:491

Table S5. Prediction skill metrics of PMCAMx-SR (sensitivity test) against AMS factor analysis during 25 February – 23 March 2009[a].

	Mean Observed ($\mu g\ m^{-3}$)	Mean Predicted ($\mu g\ m^{-3}$)	MB ($\mu g\ m^{-3}$)	MAGE ($\mu g\ m^{-3}$)	FBIAS	FERROR
			Cabauw			
OA	1.34	2.65	1.31	1.59	0.60	0.81
HOA	0.25	0.55	0.31	0.38	0.72	0.91
BBOA	0.13	1.16	1.04	1.05	1.39	1.44
OOA	0.96	0.93	-0.03	0.52	0.11	0.68
			Helsinki			
OA	2.84	3.98	1.14	1.39	0.39	0.45
HOA	0.45	0.28	-0.16	0.25	-0.14	0.66
BBOA	0.40	1.84	1.44	1.44	1.24	1.24
OOA	1.99	1.86	-0.14	0.58	-0.04	0.36
			Mace Head			
OA	1.04	0.63	-0.41	1.41	0.31	1.38
HOA	0.09	0.004	-0.09	0.09	-0.53	1.15
BBOA	0.34	0.01	-0.32	0.34	-0.38	1.24
OOA	0.61	0.62	0.004	0.98	0.38	1.37
			Melpitz			
OA	1.62	1.25	-0.36	0.94	-0.25	0.70
HOA	0.15	0.09	-0.05	0.08	-0.31	0.68
BBOA	0.18	0.41	0.23	0.31	0.76	0.96
OOA	1.29	0.75	-0.54	0.85	-0.51	0.88
			Hyytiala			
OA	1.45	2.41	0.96	1.14	0.57	0.66
HOA	0.05	0.14	0.08	0.09	0.82	0.93
BBOA	0.07	0.89	0.83	0.83	1.68	1.68
OOA	1.33	1.37	0.04	0.67	0.11	0.57
			Barcelona			
OA	8.66	3.52	-5.15	5.39	-0.69	0.79
HOA	3.53	0.21	-3.32	3.32	-1.62	1.63
BBOA	0.69	1.19	0.51	0.79	0.52	0.83
OOA	4.45	2.11	-2.34	2.56	-0.56	0.74
			Chilbolton			
OA	2.49	1.14	-1.35	1.53	-0.60	0.81
HOA	0.50	0.19	-0.32	0.32	-0.87	0.93
BBOA	0.49	0.26	-0.24	0.35	-0.66	1.03
OOA	1.49	0.69	-0.79	0.99	-0.56	0.87

[a]Number of datapoints; Cabauw: 418, Helsinki: 350, Mace Head: 206, Melpitz: 314, Hyytiala:426,Barcelona:485,Chilbolton:491

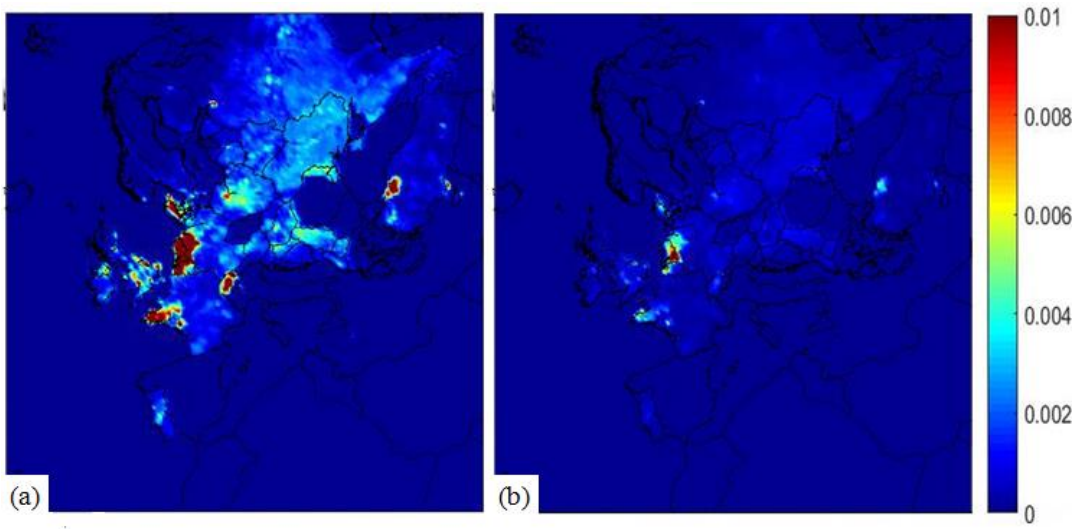

Figure S1. OA ground level emission rates (kg d^{-1} km^{-2}) spatial distribution from agricultural activities (waste burning) for (a) 1-29 May 2008 and (b) 25 February-22 March 2009. During both periods the average value of this source is approximately 7 × 10^{-3} kg d^{-1} km^{-2} and the maximum value is nearly 4 kg d^{-1} km^{-2} in the Netherlands.

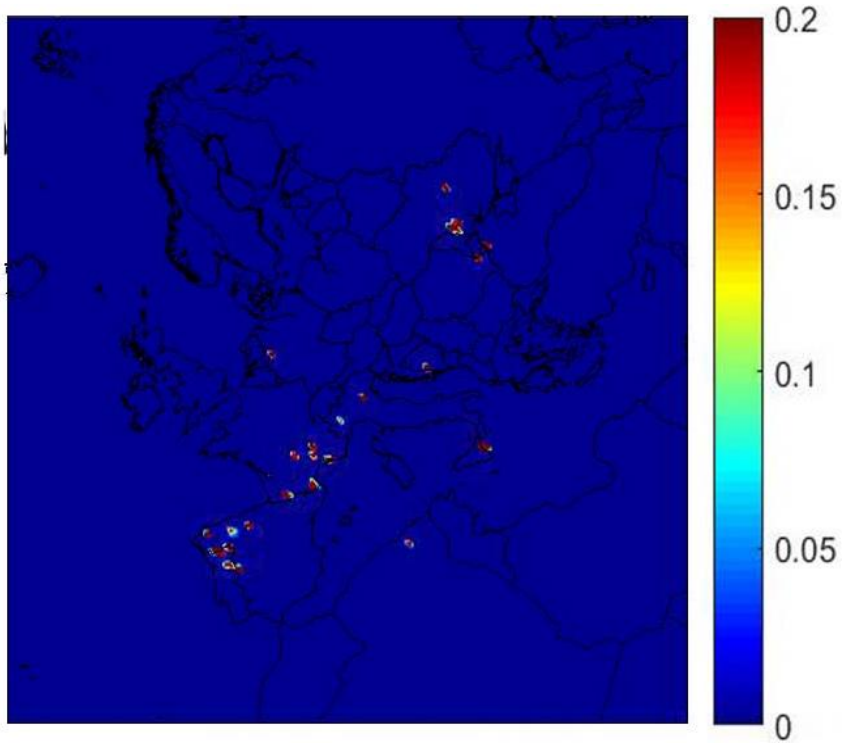

Figure S2. OA ground level emission rates (kg d^{-1} km^{-2}) spatial distribution from wildfires during 25 February-22 March 2009. Nearly 2000 tn day^{-1} are emitted in northwestern Spain and northern Portugal. The 2009 national fire data from these two countries based on the European Forest Fire Information System (EFFIS) (http://effis.jrc.ec.europa.eu) indicated intense fire activity in the second half of March driven by dry weather and strong winds.

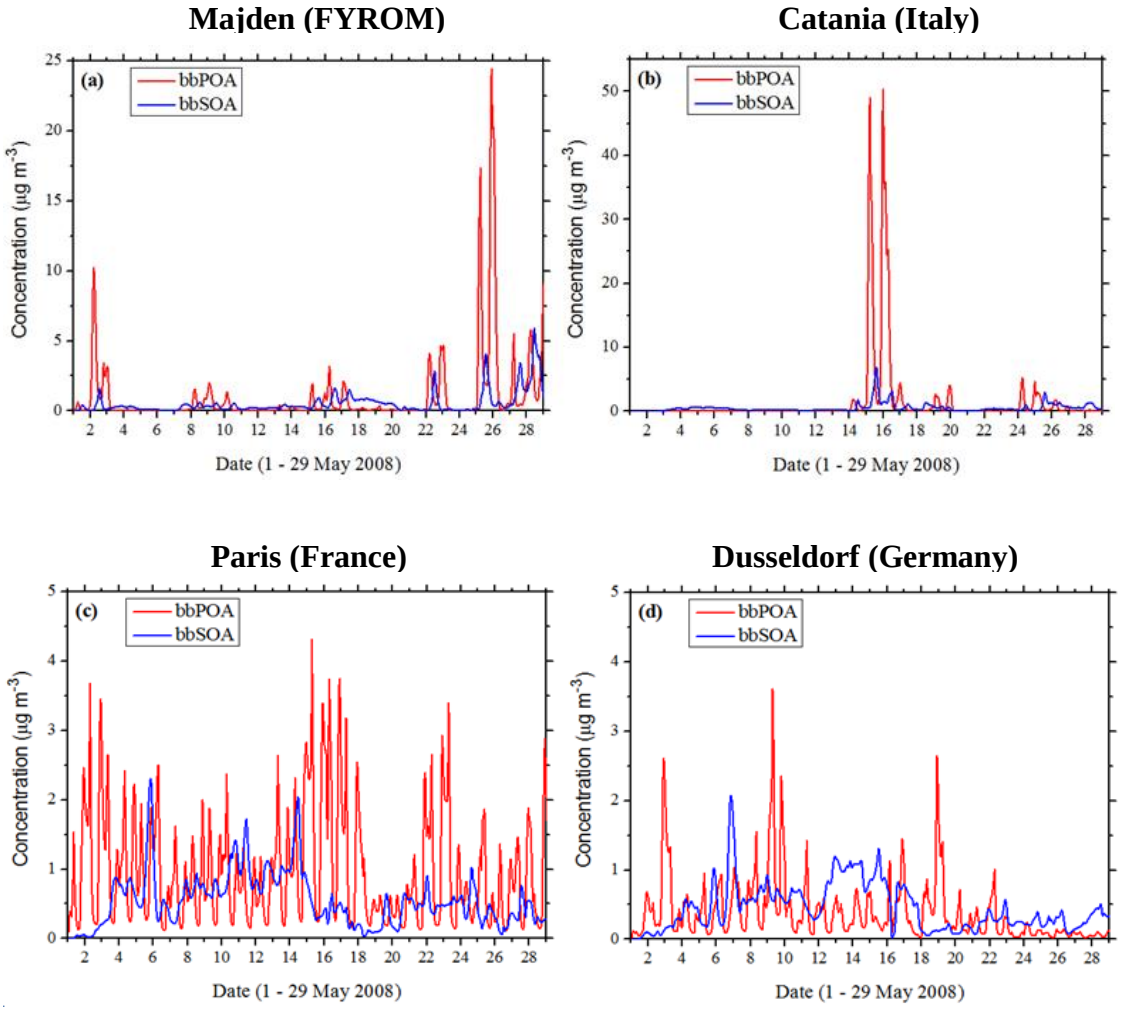

Figure S3. Timeseries of $PM_{2.5}$ bbOA concentrations in (a) Majden (FYROM), (b) Catania (Italy), (c) Paris (France) and (d) Dusseldorf (Germany) during 1-29 May 2008.

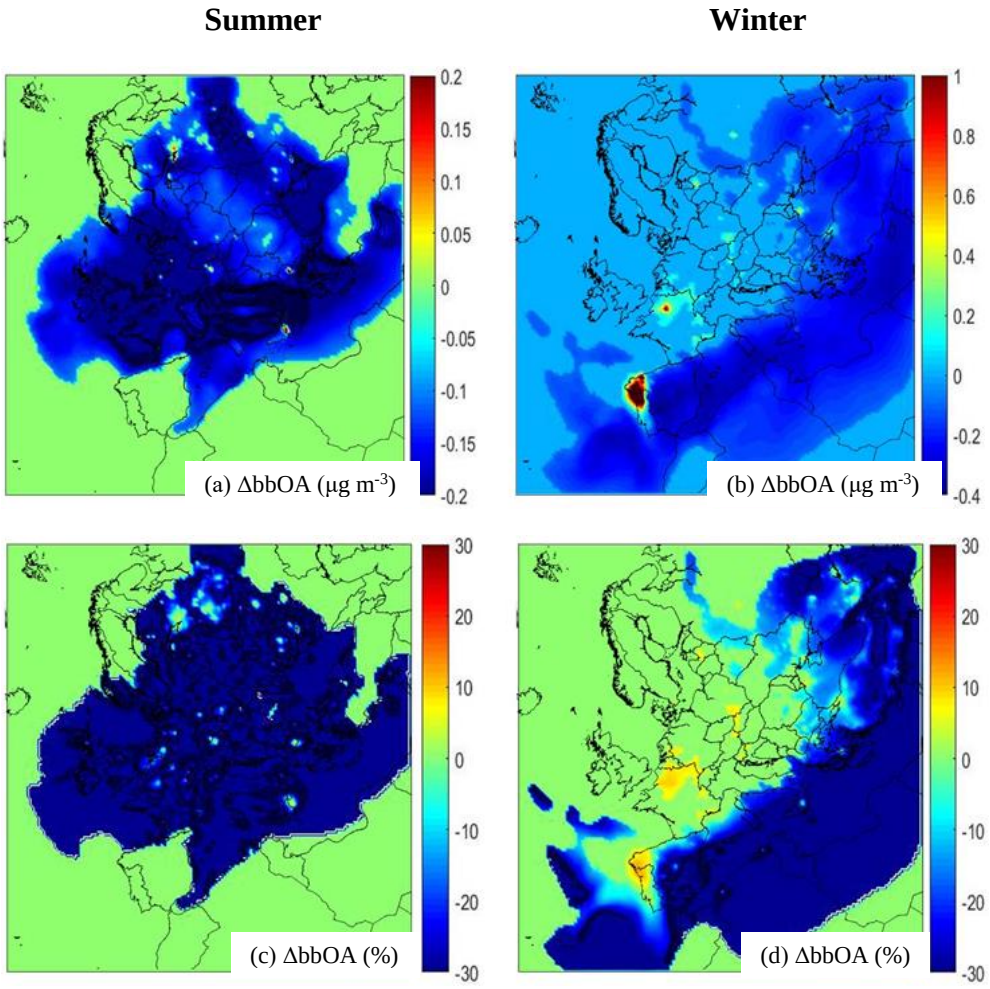

Figure S4. Average predicted absolute (μg m^{-3}) change of ground-level $PM_{2.5}$ total bbOA concentrations from PMCAMx-SR base case and sensitivity simulations during the modeled summer and winter periods (a-b). Also shown the corresponding relative (%) change of ground-level $PM_{2.5}$ total bbOA concentrations during the modeled periods (c-d). Positive values indicate that PMCAMx-SR sensitivity run predicts higher concentrations.