atmosphere

Supplementary material

Sources and Geographical Origins of PM_{10} in Metz (France) Using Oxalate as a Marker of Secondary Organic Aerosols by Positive Matrix Factorization Analysis

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Received: 31 May 2019; Accepted: 1 July 2019; Published: date

Table S1. Time series comparison of PMF factors before and after constrains. Correlation coefficient (r^2) for all profiles are higher than 0.96, intercepts were all 0.

	Time series
Primary Traffic	1.06 (r^2=0.98)
Wood-Burning	0.92 (r^2=0.98)
Dust	0.86 (r^2=1)
Primary Bio.	1.91 (r^2=0.99)
Secondary Marine Bio.	1.02 (r^2=1)
Oxalate-rich	1.04 (r^2=1)
Sulfate-rich	0.76 (r^2=0.98)
Nitrate-rich	1.22 (r^2=1)
Aged Sea Salt	0.97 (r^2=1)

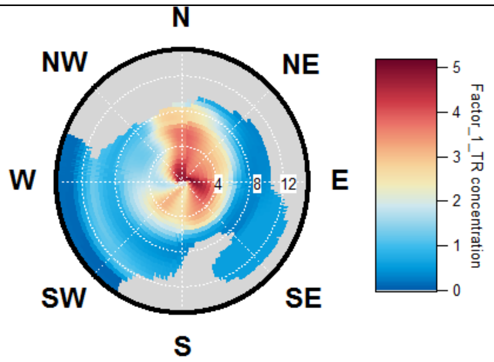
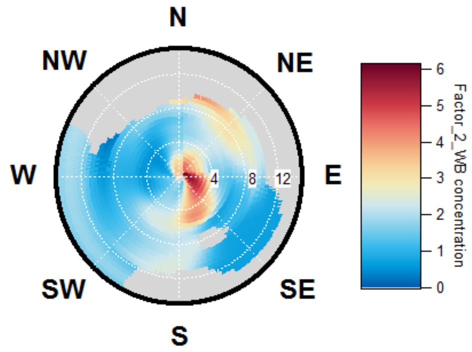
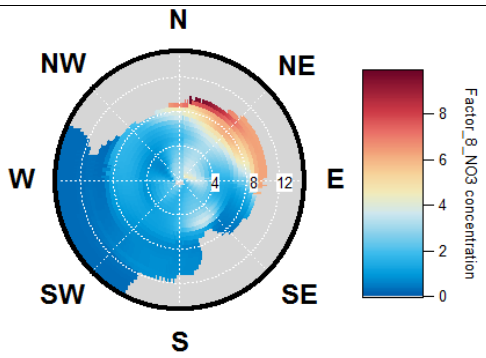
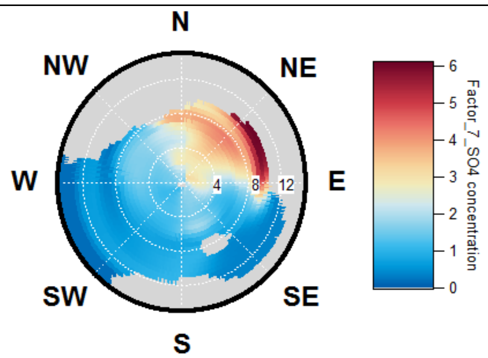
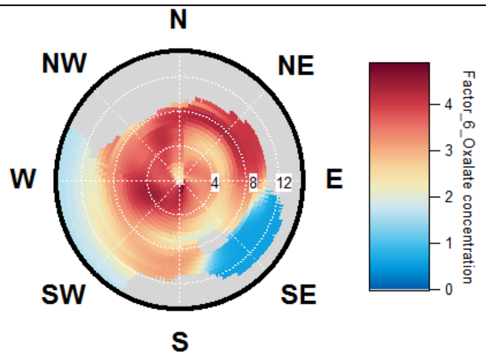
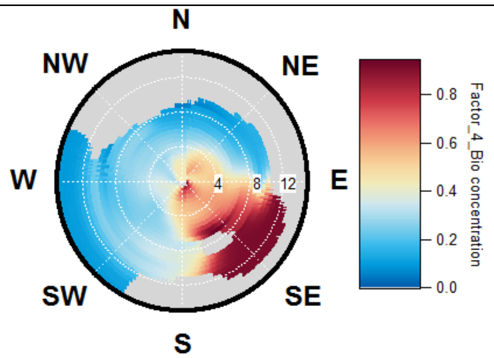
Table S2. Mapping results of the bootstrap analysis after constrains implementation, in comparison with the unconstrained bootstrap run (in parenthesis). F1: Traffic, F2: Wood-burning, F3: Dust, F4: Primary Biogenic, F5: Secondary Marine Biogenic, F6: Oxalate-rich, F7: Sulfate-rich, F8: Nitrate-rich, F9: Aged Sea Salt.

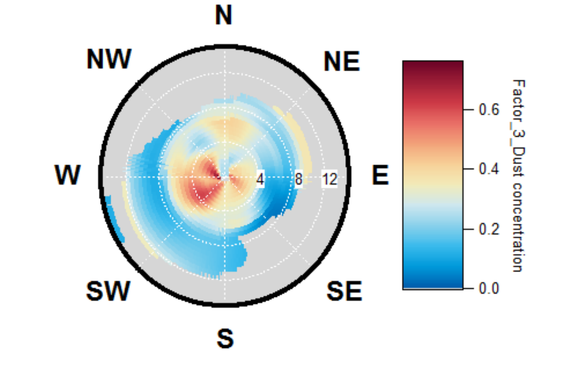
	F1	**F2**	**F3**	**F4**	**F5**	**F6**	**F7**	**F8**	**F9**
Boot F1	100 (98)	0 (2)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
Boot F2	0 (0)	100 (100)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
Boot F3	0 (0)	0 (0)	100 (100)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
Boot F4	0 (0)	0 (0)	0 (0)	100 (100)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
Boot F5	0 (0)	0 (1)	0 (0)	0 (0)	100 (99)	0 (0)	0 (0)	0 (0)	0 (0)
Boot F6	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	100 (100)	0 (0)	0 (0)	0 (0)
Boot F7	0 (2)	0 (2)	0 (1)	0 (0)	0 (0)	6 (6)	94 (79)	0 (2)	0 (0)
Boot F8	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	100 (100)	0 (0)
Boot F9	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	100 (100)

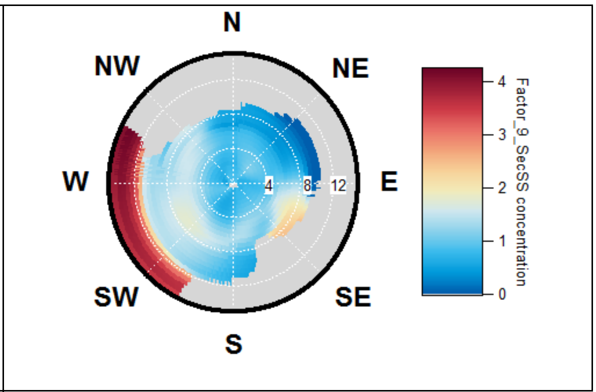
Non-parametric Wind Regression (Henry et al., 2009) consists in coupling atmospheric concentrations of a given pollutant with wind data (speed and wind direction), using the equation herein below.

$$E(\theta|\vartheta) = \frac{\sum_{i=1}^{N} K_1\left(\frac{\theta - W_i}{h}\right) \cdot K_2\left(\frac{\vartheta - Y_i}{u}\right) \cdot C_i}{\sum_{i=1}^{N} K_1\left(\frac{\theta - W_i}{h}\right) \cdot K_2\left(\frac{\vartheta - Y_i}{u}\right)}$$

where W_i, Y_i and C_i are respectively the wind direction, wind speed and concentration measured at t_i; θ and ϑ are the modelled wind direction and wind speed; h and u are two smoothing variables; and K_1 and K_2 are two Kernel functions (respectively Gaussian and Epanechnikov). NWR is therefore a weighing average, where the weighing coefficients are determined through Kernel functions, in order to give weight to C_i values where W_i and Y_i are close respectively to θ and ϑ.

Primary Traffic	Wood-burning
	
Nitrate-rich	Sulfate-rich
	
Oxalate-rich	Primary Biogenic
	
Dust	Aged Sea Salt





Secondary Marine Biogenic Aerosols

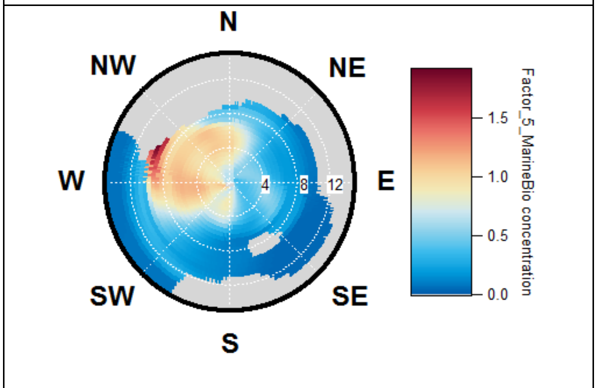


Figure S1. Non-parametric Wind Regression analysis applied to the PMF timeseries. Radial axis is relative to the wind speed (km/h), color to the concentrations (μg/m³).

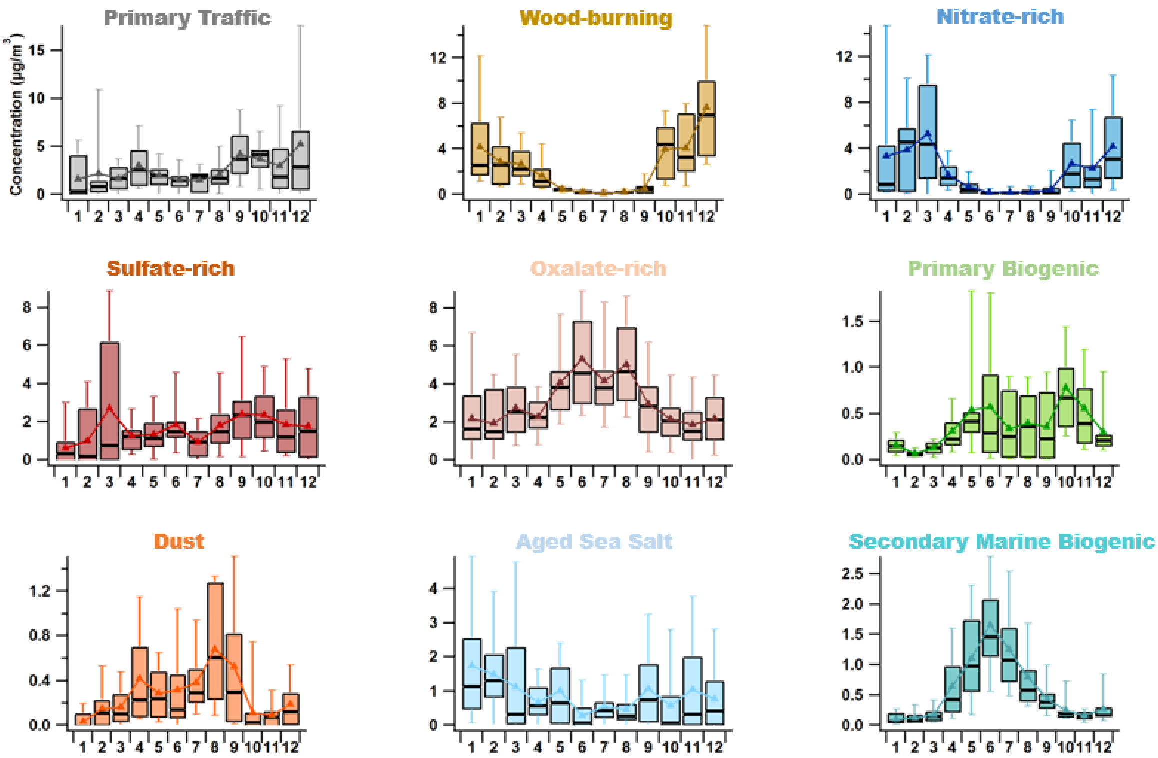


Figure S2. Monthly box and whiskers distribution (10th, 25th, 50th, 75th and 90th have been used) of the 9 PMF factors. Triangle markers correspond to the monthly mean values.

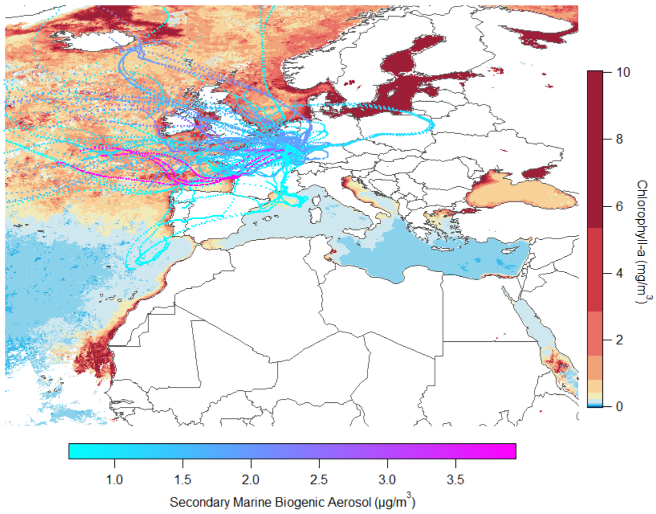


Figure S3. Mean Chlorophyll-a concentrations (mg/m³) over May and June 2015 from MODIS observations; corresponding backtrajectories during the same period, color-coded by Secondary Marine Biogenic Aerosol concentration (µg/m³).

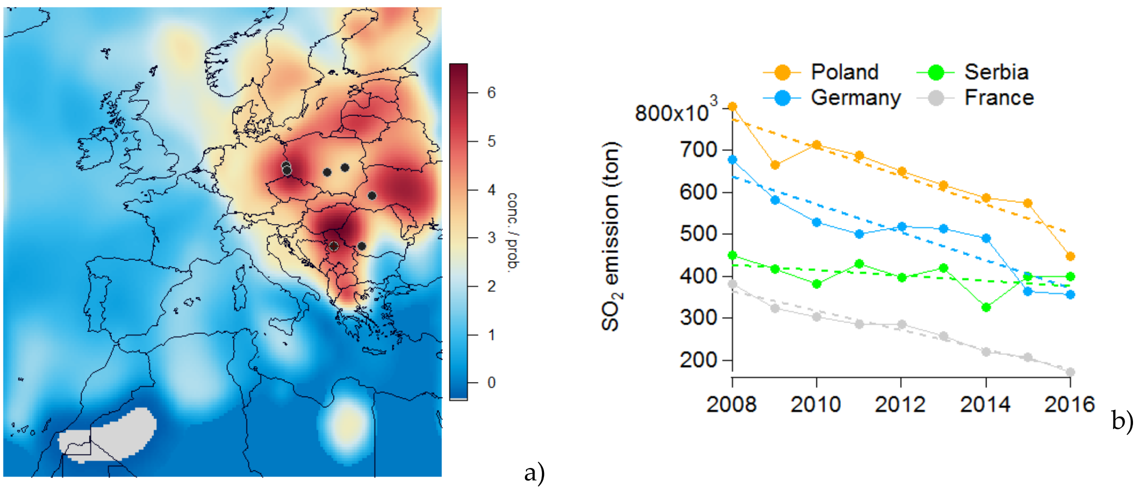


Figure S4. (a) CWT analysis for the SO_4-rich factor, with locations of selected coal-powered power plants in Eastern Europe, with energy production higher than 2000 MWh. (b) SO_2 emissions (in ton) for Poland, Serbia, Germany and France from 2008 to 2016 (data available at https://ec.europa.eu/eurostat/data/database).