Characterization and source apportionment of particulate matter and associated culturable bacterial bioaerosols at sites cultivating aromatic and medicinal plants

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Supplementary material

SI 1 Sample collection

The biological aerosol samples were collected using polycarbonate (PC) filters (37 mm diameter, 0.4 μm pore size) fitted in filter holders. Each sampling event lasted for 8 hours per day at a flow rate of 12.5 L/min, conducted at a height of ~2 m above ground level. Sampling was carried out on 15 non-consecutive days at each site (a total of 45 samples) during the study period.

In this study, samples were collected five days per week over a three-week period, resulting in a total of 45 samples. For analysis and presentation, each week was treated as a separate sampling phase (referred to as first, second, and third sampling, respectively). The data shown in the graphs represent the average of five daily samples from each week.

SI 2 Quality Control

Quality control of metals and ions was conducted using the analysis of blanks, calibration curves, accuracy, recovery, and precision.

Element	LOD (mg/L)	Accuracy (%)	RSD (%)
Al	0.02	4.1	1.1
B	0.0005	5.4	1.4
Ba	0.0005	5.5	1.4
Ca	0.0005	3.6	1.2
Cu	0.005	4.9	0.7
Fe	0.005	3.7	0.5
K	0.10	5.1	1.8
Mg	0.0005	3.2	1.3
Mn	0.001	4.5	0.9
Zn	0.005	2.2	1.2
Pb	0.006	4.17	1.65
Cd	0.0054	4.2	1.13
As	0.001	5.1	1.38

Analyte	LOD (mg/L)	LOQ (mg/L)	RSD (%)	Accuracy (%)
K^+	0.03	0.10	2.1	83.8
Na^+	0.006	0.02	0.60	95.2
Li^+	0.002	0.006	0.31	94.7
Mg^{2+}	0.004	0.01	0.50	90.5
NH_4^+	0.003	0.01	0.51	91.4
Ca^{2+}	0.01	0.03	0.85	86.8
F^-	0.07	0.21	1.77	89.6
Br^-	0.07	0.22	2.19	81.0
Cl^-	0.09	0.27	2.34	90.3
NO_3^-	0.09	0.28	2.34	86.7
NO_2^-	0.04	0.14	3.93	80.0
PO_4^{3-}	0.40	0.12	4.54	84.3
SO_4^{2-}	0.29	0.88	4.94	80.6

SI 3 Positive matrix factorization

Positive Matrix Factorization (PMF) is a multivariate statistical method widely used for identifying and apportioning pollution sources. In this study (Al, B, Ba, Ca, Cd, Co, Cr, Cu, Fe, K, Li, Mg, Mn, Ni, Pb, and Zn) elements and heavy metals, and anionic (F^-, Cl^-, Br^-, NO_3^-, and SO_4^{2-}) and cationic components (Na^+, NH_4^+, K^+, Mg^{2+} and Ca^{2+}) were included for PM source apportionment. The U.S. PMF 5.0 software was employed for a preliminary source apportionment analysis [1]. PMF relies on measured data values and their associated uncertainties,

without requiring previous knowledge of the exact emission profiles of individual pollutants. It can determine the contributions of different pollution sources by analyzing observations at the receptor site and the PMF can be expressed by equation 2;

$$X_{ij} = \sum_{k=1}^{\bar{p}} g_{ik} f_{kj} + e_{ij} \tag{2}$$

Where i and j are the number of samples and chemical species; p represents the number of sources; eij denotes the residual for each sample; g is the mass contribution and f is the source profile [2]. The model resulted in an optimum solution-based objective function (minimizing Q), as given by equation 3;

$$Q = \sum_{i=1}^{n} \sum_{j=1}^{m} \left[\frac{x_{ij} - \sum_{k=1}^{\bar{p}} g_{ik} f_{kj}}{u_{ij}} \right]^2 \tag{3}$$

To initiate the PMF 5.0 model, two input files, concentration values and uncertainty values for each species, are required. The uncertainties were calculated with the following equation (MDL is the method detection limit; c is the concentration of chemical species, and error fraction is the percent of measurement uncertainty) as given in Equation.

$$U_{nc} = \begin{cases} MDL \times \frac{5}{6}, & c \leq MDL \\ \sqrt{MDL^2 + (Error\ fraction \times c)^2}, & c \geq MDL \end{cases}$$

SI 4

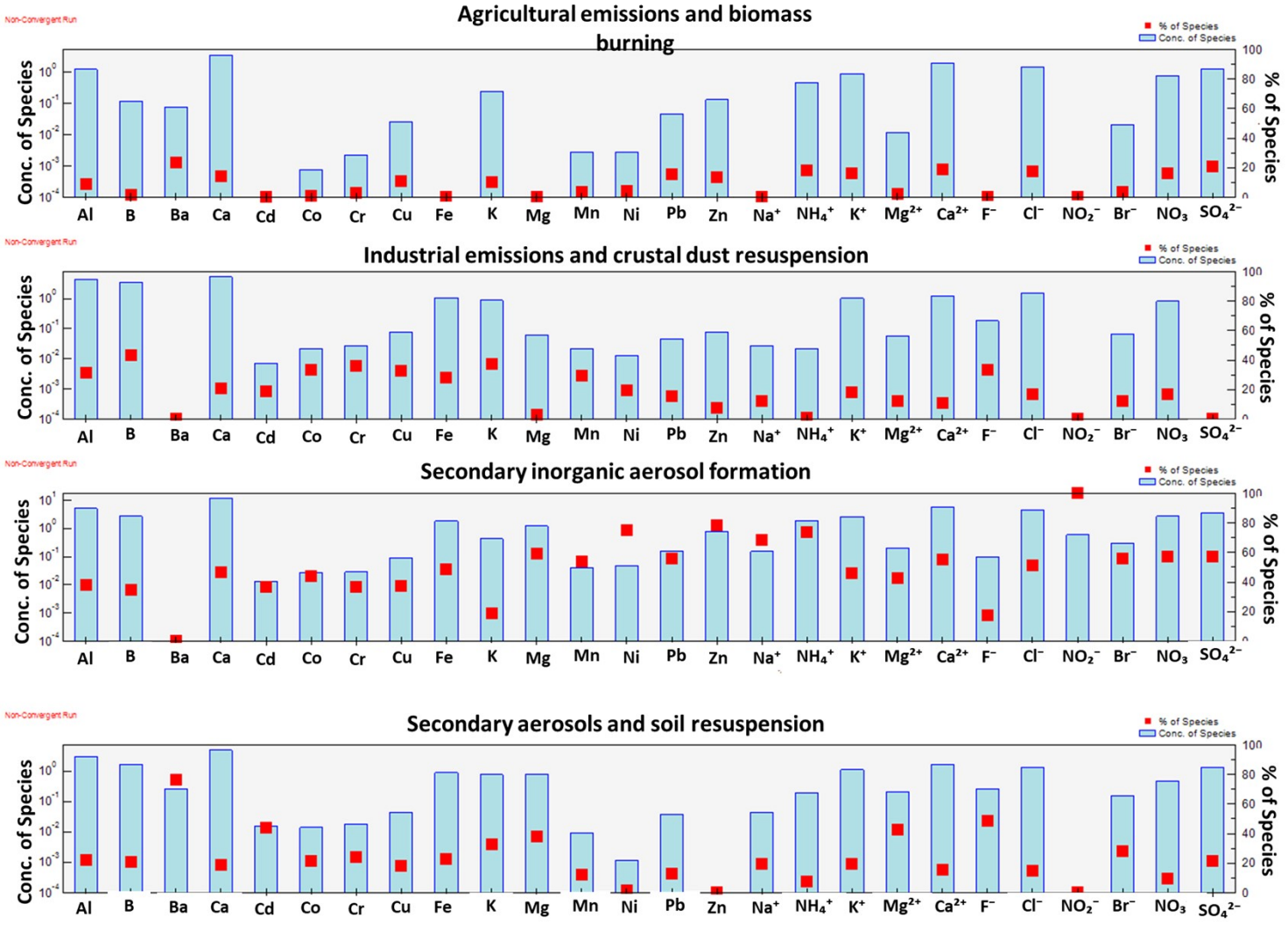

Figure SI 4 -Source profiles of elements and ions in $PM_{2.5}$ obtained through positive matrix factorisation (PMF) analysis.

SI 5

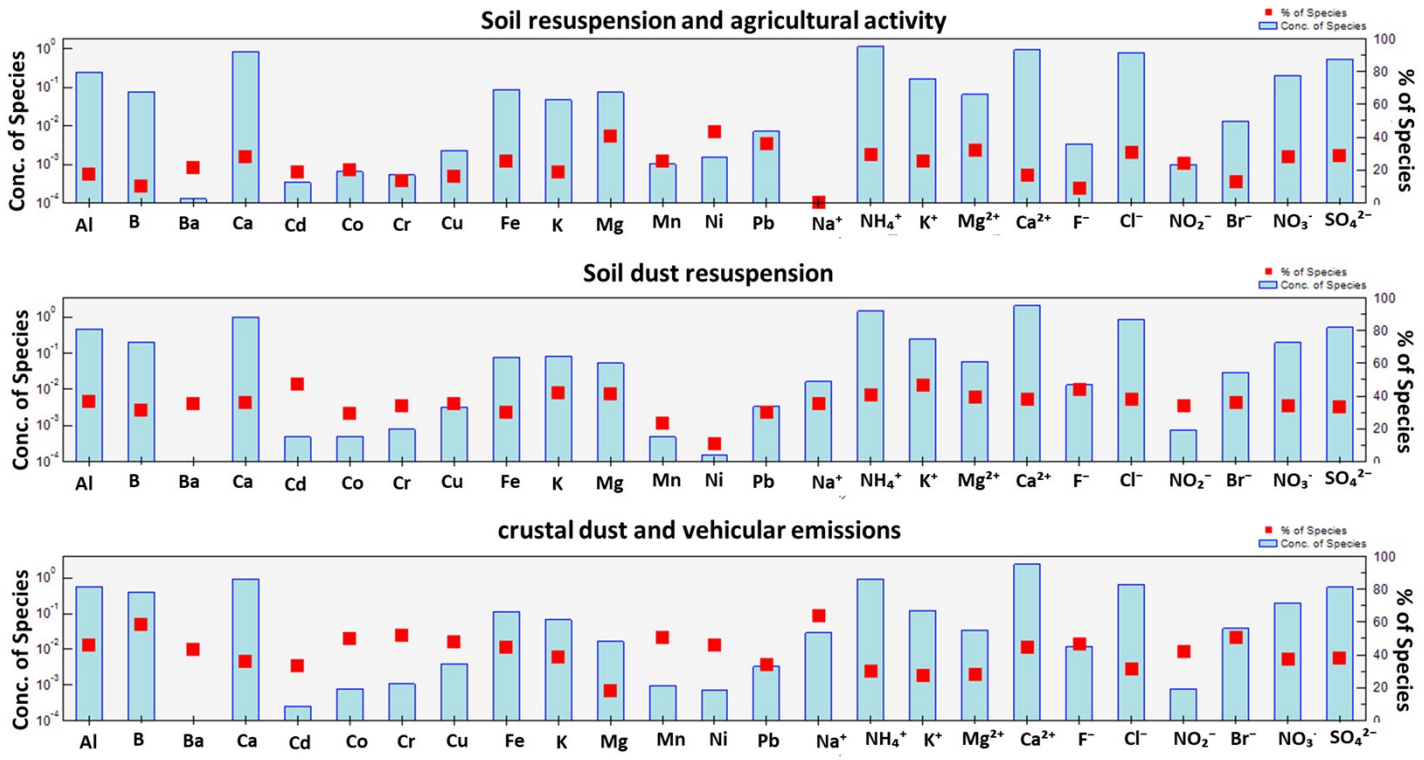

Figure SI 5 -Source profiles of elements and ions in PM_{10} obtained through positive matrix factorisation (PMF) analysis

References

1 USEPA, 2014. Positive Matrix Factorization (PMF) 5.0 Fundamentals & User Guide. Office of Research and Development

2 G. Norris, R. Duvall, S. Brown and S. Bai, EPA positive matrix factorization (PMF) 5.0 fundamentals and user guide, US Environmental Protection Agency, Washington, DC, www2. epa. gov/sites/production/files/2015-02/documents/pmf_5. 0_user_guide. pdf, 2014.