

Supplementary Materials

A Comparison of Multiply Combined Models: Including PCA/MLR-CMB, Unmix-CMB and PMF-CMB Models, for Source Apportionment

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Table S1. Seven actual PM₁₀ source profiles measured in Anyang city

Species	resuspended	soil	coal	cement	vehicle	secondary sulfate	secondary nitrate
Na	0.37	0.28	0.46	0.25	1.04	0.00	0.00
Mg	1.56	1.72	0.70	2.15	0.09	0.00	0.00
Al	6.91	7.40	14.75	3.82	3.65	0.00	0.00
Si	21.24	26.24	19.45	10.95	7.22	0.00	0.00
P	0.12	0.10	0.12	0.04	0.95	0.00	0.00
K	1.73	2.43	1.21	1.20	0.87	0.00	0.00
Ca	9.33	5.35	5.22	29.72	0.01	0.00	0.00
Ti	0.46	0.49	0.64	0.13	0.02	0.00	0.00
V	0.01	0.01	0.02	0.00	0.01	0.00	0.00
Cr	0.01	0.01	0.01	0.01	0.02	0.00	0.00
Mn	0.07	0.08	0.04	0.03	4.26	0.00	0.00
Fe	6.16	4.31	4.63	1.59	0.01	0.00	0.00
Co	0.00	0.00	0.00	0.00	0.01	0.00	0.00
Ni	0.00	0.01	0.01	0.01	0.02	0.00	0.00
Cu	0.01	0.01	0.02	0.00	0.06	0.00	0.00
Zn	0.12	0.02	0.03	0.07	0.00	0.00	0.00
Br	0.11	0.06	0.10	0.07	0.00	0.00	0.00
Ba	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pb	0.07	0.01	0.02	0.01	0.00	0.00	0.00
TC	11.43	3.58	13.93	3.29	67.41	0.00	0.00
NH ₄ ⁺	0.00	0.00	0.00	0.94	0.00	0.00	0.00
Cl ⁻	0.02	0.01	0.01	0.01	2.42	27.30	22.50
NO ₃ ⁻	0.01	0.02	0.22	0.33	0.88	0.00	0.00
SO ₄ ²⁻	0.06	0.06	0.15	0.00	1.71	0.00	77.50

Table S2. seven actual PM₁₀ source profiles measured in Taiyuan city

Species	resuspended	soil	coal	cement	vehicle	secondary sulfate	secondary nitrate
Na	0.73	0.71	0.22	0.32	1.04	0.00	0.00
Mg	1.55	1.64	0.29	3.00	0.09	0.00	0.00
Al	7.08	8.97	9.28	3.48	3.65	0.00	0.00
Si	22.33	26.10	12.36	13.08	7.22	0.00	0.00
P	0.12	0.10	0.07	0.01	0.95	0.00	0.00
K	1.09	1.68	0.56	1.11	0.87	0.00	0.00
Ca	13.70	9.12	2.78	32.69	0.01	0.00	0.00
Ti	0.35	0.42	0.68	0.11	0.02	0.00	0.00
V	0.01	0.01	0.01	0.00	0.01	0.00	0.00
Cr	0.02	0.01	0.01	0.01	0.02	0.00	0.00
Mn	0.05	0.07	0.03	0.02	4.26	0.00	0.00
Fe	3.46	4.07	1.73	0.97	0.01	0.00	0.00
Co	0.00	0.00	0.00	0.00	0.01	0.00	0.00
Ni	0.01	0.01	0.00	0.00	0.02	0.00	0.00
Cu	0.01	0.01	0.01	0.00	0.06	0.00	0.00
Zn	0.05	0.02	0.03	0.00	0.00	0.00	0.00
Br	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ba	0.06	0.06	0.03	0.01	0.00	0.00	0.00
Pb	0.02	0.01	0.01	0.00	0.00	0.00	0.00
TC	12.88	6.06	27.70	3.21	67.41	0.00	0.00
NH ₄ ⁺	0.04	0.03	0.01	0.01	2.42	27.30	22.50
Cl ⁻	0.25	0.05	0.06	0.04	0.88	0.00	0.00
NO ₃ ⁻	0.00	0.00	0.00	0.00	1.71	0.00	77.50
SO ₄ ²⁻	7.03	0.57	0.72	1.70	8.57	72.70	0.00

Table S3. seven actual PM₁₀ source profiles measured in Tianjin city

Species	resuspended	soil	coal	cement	vehicle	secondary sulfate	secondary nitrate
Na	1.26	1.85	4.18	0.93	1.04	0.00	0.00
Mg	1.45	2.05	0.76	1.96	0.09	0.00	0.00
Al	7.91	10.10	7.67	4.18	3.65	0.00	0.00
Si	17.60	22.59	17.03	9.14	7.22	0.00	0.00
P	0.11	0.11	1.64	0.02	0.95	0.00	0.00
K	2.62	3.68	1.21	2.76	0.87	0.00	0.00
Ca	6.84	8.54	3.15	37.81	0.01	0.00	0.00
Ti	0.65	0.76	0.53	0.66	0.02	0.00	0.00
V	0.00	0.00	0.02	0.00	0.01	0.00	0.00
Cr	0.01	0.01	0.03	0.01	0.02	0.00	0.00
Mn	0.04	0.06	0.09	0.02	4.26	0.00	0.00
Fe	2.39	2.96	2.74	1.44	0.01	0.00	0.00
Co	0.01	0.00	0.02	0.00	0.01	0.00	0.00
Ni	0.01	0.01	0.04	0.01	0.02	0.00	0.00
Cu	0.01	0.00	0.12	0.01	0.06	0.00	0.00
Zn	0.08	0.00	1.07	0.01	0.00	0.00	0.00
Br	0.00	0.00	0.03	0.00	0.00	0.00	0.00
Ba	0.24	0.13	0.19	0.05	0.00	0.00	0.00
Pb	0.01	0.01	0.39	0.00	0.00	0.00	0.00
TC	11.17	4.92	20.07	3.16	67.41	0.00	0.00
NH ₄ ⁺	0.02	0.01	0.28	0.00	2.42	27.30	22.50
Cl ⁻	0.02	0.01	0.13	0.00	0.88	0.00	0.00
NO ₃ ⁻	0.00	0.00	0.00	0.00	1.71	0.00	77.50
SO ₄ ²⁻	4.63	0.75	3.56	2.17	8.57	72.70	0.00

Table S4. seven actual PM₁₀ source profiles measured in Urumchi city

Species	resuspended	soil	coal	cement	vehicle	secondary sulfate	secondary nitrate
Na	0.54	0.31	0.26	0.93	1.04	0.00	0.00
Mg	0.93	1.50	0.27	1.96	0.09	0.00	0.00
Al	7.05	6.18	10.33	4.18	3.65	0.00	0.00
Si	16.26	25.35	13.61	9.14	7.22	0.00	0.00
P	0.39	0.11	0.12	0.02	0.95	0.00	0.00
K	0.80	2.21	0.58	2.76	0.87	0.00	0.00
Ca	7.32	4.91	2.34	37.81	0.01	0.00	0.00
Ti	0.44	0.45	0.63	0.66	0.02	0.00	0.00
V	0.01	0.01	0.01	0.00	0.01	0.00	0.00
Cr	0.01	0.01	0.01	0.01	0.02	0.00	0.00
Mn	0.05	0.11	0.03	0.02	4.26	0.00	0.00
Fe	2.30	3.59	2.95	1.44	0.01	0.00	0.00
Co	0.01	0.00	0.00	0.00	0.01	0.00	0.00
Ni	0.01	0.00	0.00	0.01	0.02	0.00	0.00
Cu	0.01	0.01	0.01	0.01	0.06	0.00	0.00
Zn	0.02	0.02	0.03	0.01	0.00	0.00	0.00
Br	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ba	0.25	0.07	0.04	0.05	0.00	0.00	0.00
Pb	0.01	0.00	0.02	0.00	0.00	0.00	0.00
TC	19.24	4.05	30.73	3.16	67.41	0.00	0.00
NH ₄ ⁺	0.03	0.02	0.05	0.00	2.42	27.30	22.50
Cl ⁻	0.03	0.06	0.05	0.00	0.88	0.00	0.00
NO ₃ ⁻	0.00	0.03	0.00	0.00	1.71	0.00	77.50
SO ₄ ²⁻	1.54	0.63	1.02	2.17	8.57	72.70	0.00

Table S5. seven actual PM₁₀ source profiles measured in Yinchuan city

Species	resuspended	soil	coal	cement	vehicle	secondary sulfate	secondary nitrate
Na	0.82	0.89	0.76	0.60	1.04	0.00	0.00
Mg	2.80	2.04	1.86	1.54	0.09	0.00	0.00
Al	8.67	5.70	5.47	3.40	3.65	0.00	0.00
Si	15.88	24.43	23.96	14.65	7.22	0.00	0.00
P	0.67	0.10	0.14	0.05	0.95	0.00	0.00
K	0.65	1.95	2.11	1.35	0.87	0.00	0.00
Ca	8.50	9.61	8.49	18.48	0.01	0.00	0.00
Ti	0.41	0.36	0.26	0.14	0.02	0.00	0.00
V	0.01	0.01	0.01	0.00	0.01	0.00	0.00
Cr	0.01	0.01	0.01	0.00	0.02	0.00	0.00
Mn	0.10	0.06	0.05	0.02	4.26	0.00	0.00
Fe	4.50	3.09	2.28	3.01	0.01	0.00	0.00
Co	0.00	0.00	0.00	0.00	0.01	0.00	0.00
Ni	0.00	0.00	0.01	0.00	0.02	0.00	0.00
Cu	0.01	0.00	0.00	0.00	0.06	0.00	0.00
Zn	0.01	0.01	0.03	0.05	0.00	0.00	0.00
Br	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ba	0.20	0.04	0.04	0.03	0.00	0.00	0.00
Pb	0.01	0.01	0.01	0.01	0.00	0.00	0.00
TC	6.74	2.01	12.63	9.16	67.41	0.00	0.00
NH ₄ ⁺	0.04	0.00	0.01	0.00	2.42	27.30	22.50
Cl ⁻	0.25	0.09	0.06	0.14	0.88	0.00	0.00
NO ₃ ⁻	0.00	0.00	0.00	0.00	1.71	0.00	77.50
SO ₄ ²⁻	7.03	1.14	0.72	1.06	8.57	72.70	0.00

Table S6. Factor loadings of Dataset A, by PCA/MLR. (The bold values were the markers in the corresponding factor.)

Species	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6
Na	0.12	0.28	0.68	0.02	-0.10	0.35
Mg	0.83	0.08	0.17	0.09	0.18	0.06
Al	0.95	0.18	0.15	-0.03	0.07	0.01
Si	0.97	0.19	0.05	-0.01	0.05	-0.03
P	0.44	0.73	0.03	0.20	0.12	0.23
K	0.96	0.22	0.08	0.00	0.04	-0.04
Ca	0.95	0.07	0.10	-0.06	0.06	0.01
Ti	0.98	0.09	0.06	-0.02	0.07	-0.01
V	0.32	-0.24	0.21	-0.07	0.40	0.23
Cr	0.38	0.33	0.38	0.04	0.35	-0.04
Mn	0.13	0.94	-0.04	0.12	-0.07	-0.02
Fe	0.97	0.10	0.05	0.00	0.09	0.04
Co	0.14	0.00	0.12	-0.06	0.79	-0.04
Ni	0.07	0.13	0.40	-0.20	0.64	0.32
Cu	-0.02	-0.05	0.04	0.00	0.30	0.70
Zn	0.08	0.06	0.75	-0.09	0.16	0.20
Br	0.78	0.12	0.15	-0.07	0.03	0.18
Ba	0.18	-0.14	0.69	0.08	0.17	0.04
Pb	0.11	-0.18	0.59	0.22	0.30	-0.19
TC	0.46	0.84	0.02	0.08	0.02	-0.04
NH ₄ ⁺	-0.03	0.24	0.22	0.89	-0.16	-0.04
Cl ⁻	0.14	0.11	0.37	0.11	-0.25	0.71
NO ₃ ⁻	-0.10	-0.06	-0.29	0.74	0.09	0.27
SO ₄ ²⁻	0.04	0.38	0.31	0.66	-0.24	-0.19
Eigenvalue	7.64	2.85	2.69	2.00	1.79	1.54
Variance %	31.84	11.86	11.20	8.32	7.47	6.43
	Mixed source 1	Vehicle exhaust		Mixed source 2		

TC: total carbon

Table S7. Predicted profiles and contributions ($\mu\text{g}/\text{m}^3$) of sources extracted by PCA/MLR model, for Dataset A

Species	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6
Na	0.38	0.72	1.02	0.11	-0.22	0.64
Mg	2.07	0.16	0.20	0.29	0.30	0.09
Al	11.81	1.79	0.88	-0.49	0.63	0.05
Si	27.52	4.35	0.65	-0.23	1.06	-0.50
P	0.22	0.30	0.01	0.14	0.04	0.06
K	2.18	0.41	0.09	-0.01	0.06	-0.05
Ca	13.00	0.82	0.65	-1.07	0.60	0.04
Ti	0.61	0.05	0.02	-0.02	0.03	0.00
V	0.02	-0.01	0.01	-0.01	0.02	0.01
Cr	0.01	0.01	0.01	0.00	0.01	0.00
Mn	0.22	1.33	-0.03	0.29	-0.08	-0.02
Fe	6.40	0.52	0.15	0.00	0.40	0.14
Co	0.02	0.00	0.01	-0.01	0.07	0.00
Ni	0.00	0.01	0.01	-0.02	0.03	0.01
Cu	-0.03	-0.05	0.02	0.01	0.24	0.46
Zn	0.04	0.03	0.21	-0.07	0.07	0.07
Br	0.15	0.02	0.01	-0.02	0.00	0.02
Ba	0.05	-0.03	0.09	0.03	0.03	0.01
Pb	0.03	-0.04	0.08	0.08	0.06	-0.03
TC	14.72	21.75	0.26	3.45	0.45	-0.76
NH ₄ ⁺	-0.21	1.33	0.72	8.33	-0.77	-0.14
Cl ⁻	0.19	0.12	0.23	0.21	-0.23	0.55
NO ₃ ⁻	-0.95	-0.46	-1.34	9.86	0.60	1.52
SO ₄ ²⁻	0.68	4.80	2.25	13.93	-2.55	-1.69
Source categories	Mixed source 1	Vehicle exhaust	noise	Mixed source 2	noise	noise
Predicted Contributions	131.90	41.33	11.12	32.48	7.99	2.56
Simulated Contributions	139.96 ^a	40.00		30.00 ^b		

^a the value is equal to the sum of simulated contributions of RD, soil dust, coal combustion and cement

^b the value is equal to the sum of simulated contributions of secondary sulfate and nitrate.

Table S8. Predicted profiles and contributions ($\mu\text{g}/\text{m}^3$) of sources extracted by Unmix model, for Dataset A

Species	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6
Na	0.80	0.98	1.53	-0.84	0.34	-0.57
Mg	1.74	-0.18	0.00	0.29	0.41	0.45
Al	10.70	-1.01	1.67	-0.39	2.85	1.26
Si	24.40	-2.73	3.33	-2.16	8.14	1.60
P	0.33	0.13	0.15	-0.19	0.45	-0.20
K	2.06	-0.12	0.29	-0.24	0.76	0.07
Ca	11.20	-1.80	1.39	0.51	2.47	1.68
Ti	0.52	-0.09	0.05	0.01	0.12	0.08
V	0.02	-0.01	0.00	0.02	0.00	0.02
Cr	0.02	0.00	0.00	0.00	0.01	0.00
Mn	0.93	0.68	0.65	-1.19	1.83	-1.05
Fe	5.33	-0.92	0.41	0.38	1.22	0.78
Co	0.00	-0.05	0.00	0.05	0.00	0.09
Ni	0.00	-0.01	0.02	0.02	0.00	0.02
Cu	-0.11	-0.07	-0.06	0.89	-0.01	0.02
Zn	0.07	0.04	0.30	-0.02	-0.06	0.06
Br	0.13	-0.02	0.03	0.01	0.02	0.01
Ba	0.06	0.04	-0.07	0.09	-0.14	0.14
Pb	0.06	0.05	-0.09	0.04	-0.01	0.13
TC	24.20	8.55	11.00	-18.40	30.50	-13.20
NH ₄ ⁺	3.40	4.88	0.30	-3.97	8.54	-3.86
Cl ⁻	0.41	0.46	0.30	-0.01	0.41	-0.43
NO ₃ ⁻	2.45	4.78	-1.98	-2.44	10.00	-3.66
SO ₄ ²⁻	8.20	9.21	2.39	-9.28	16.70	-8.10
Source categories	Mixed source 1	noise	noise	noise	Mixed source 2	noise
Predicted Contributions	140.70	14.15	25.93	-30.26	90.19	-11.72
Simulated Contributions	139.96 ^a	40.00			70.00 ^b	

^a the value is equal to the sum of simulated contributions of RD, soil dust, coal combustion and cement

^b the value is equal to the sum of simulated contributions of vehicle exhaust as well as secondary sulfate and nitrate.

Table S9. Predicted profiles and contributions ($\mu\text{g}/\text{m}^3$) of sources extracted by PMF model (F_{peak} = 0), for Dataset A

Species ^c	Factor 1	Factor 2	Factor 3
Na	0.69	0.54	0.34
Mg	1.81	0.43	0.30
Al	10.58	2.62	1.77
Si	23.76	5.83	2.80
P	0.23	0.30	0.10
K	1.97	0.60	0.26
Ca	11.48	2.02	1.71
Ti	0.53	0.09	0.07
V	0.02	0.00	0.01
Cr	0.02	0.01	0.01
Mn	0.36	1.16	0.15
Fe	5.40	1.02	0.67
Ni	0.01	0.01	0.02
Cu	0.01	0.01	0.53
Zn	0.09	0.01	0.20
Br	0.13	0.02	0.02
Pb	0.03	0.05	0.03
TC	16.81	20.11	3.80
NH ₄ ⁺	1.07	6.24	1.56
Cl ⁻	0.14	0.41	0.33
NO ₃ ⁻	0.44	5.21	1.76
SO ₄ ²⁻	2.10	12.70	2.99
Source categories	Mixed source 1	Mixed source 2	noise
Predicted Contributions	120.91	65.40	26.83
Simulated Contributions	139.96 ^a	70.00 ^b	

^a the value is equal to the sum of simulated contributions of RD, soil dust, coal combustion and cement

^b the value is equal to the sum of simulated contributions of vehicle exhaust as well as secondary sulfate and nitrate.

^c some species with low concentrations were not introduced into the PMF model.

Table S10. The calculated uncertainties of some tracers at CMB stage, for final result of Dataset A

Species	Mixed source 1			Mixed source 2		
	PCA/MLR-CMB	PMF-CMB	Unmix-CMB	PCA/MLR-CMB	PMF-CMB	Unmix-CMB
Al	0.77	0.80	0.65			
Si	1.04	0.98	0.89			
Ca	2.21	2.22	1.87			
TC						
NO ₃ ⁻				1.00	0.47	0.93
SO ₄ ²⁻				1.42	1.03	1.33

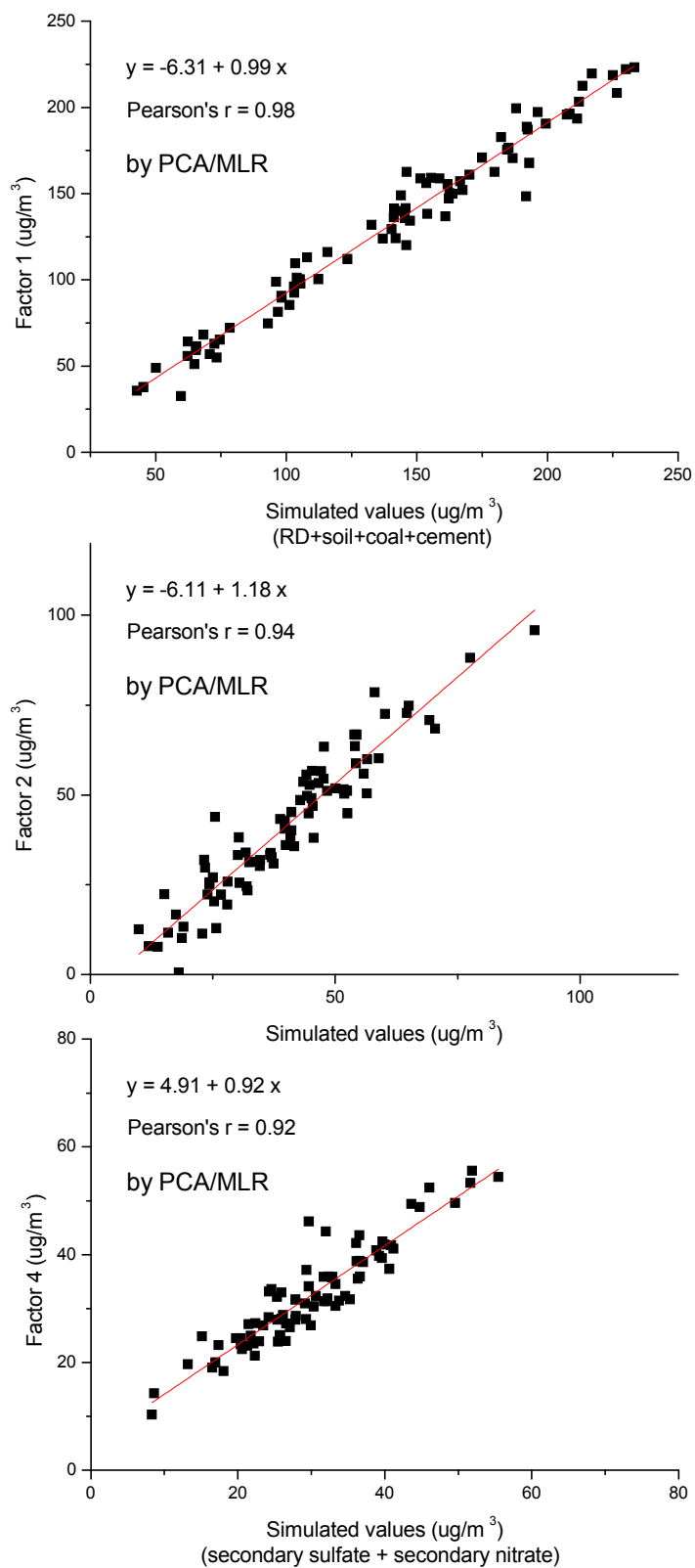


Fig. S1 The estimated contributions of factors vs. true values, by PCA/MLR

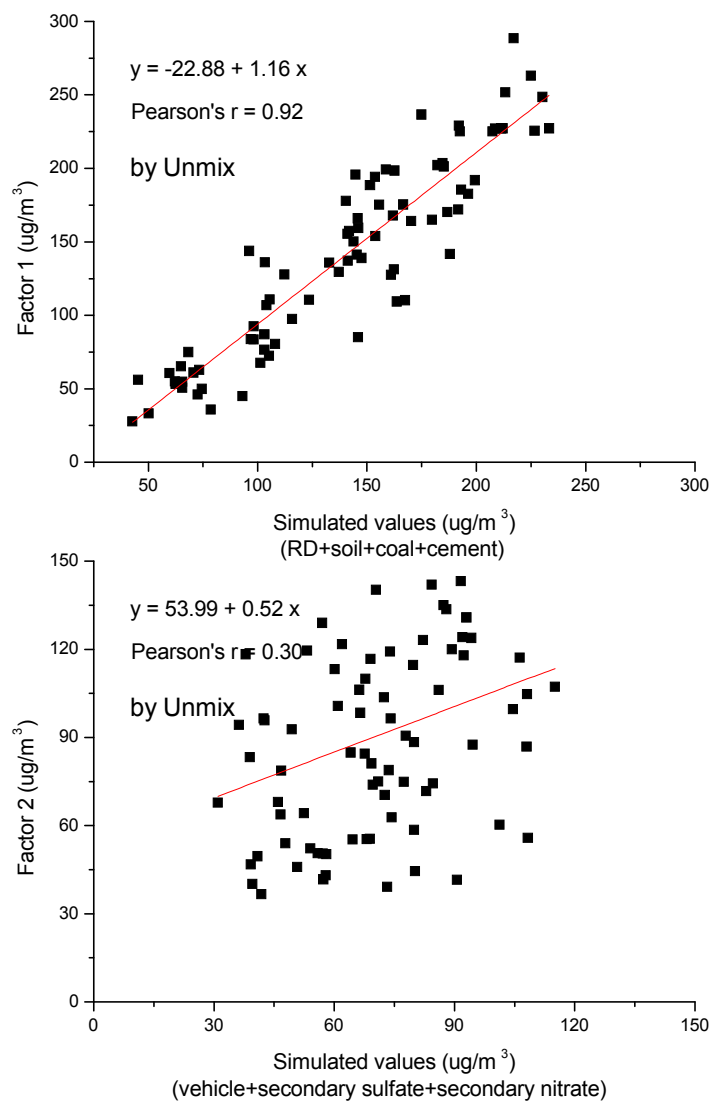


Fig. S2 The estimated contributions of factors vs. true values, by Unmix

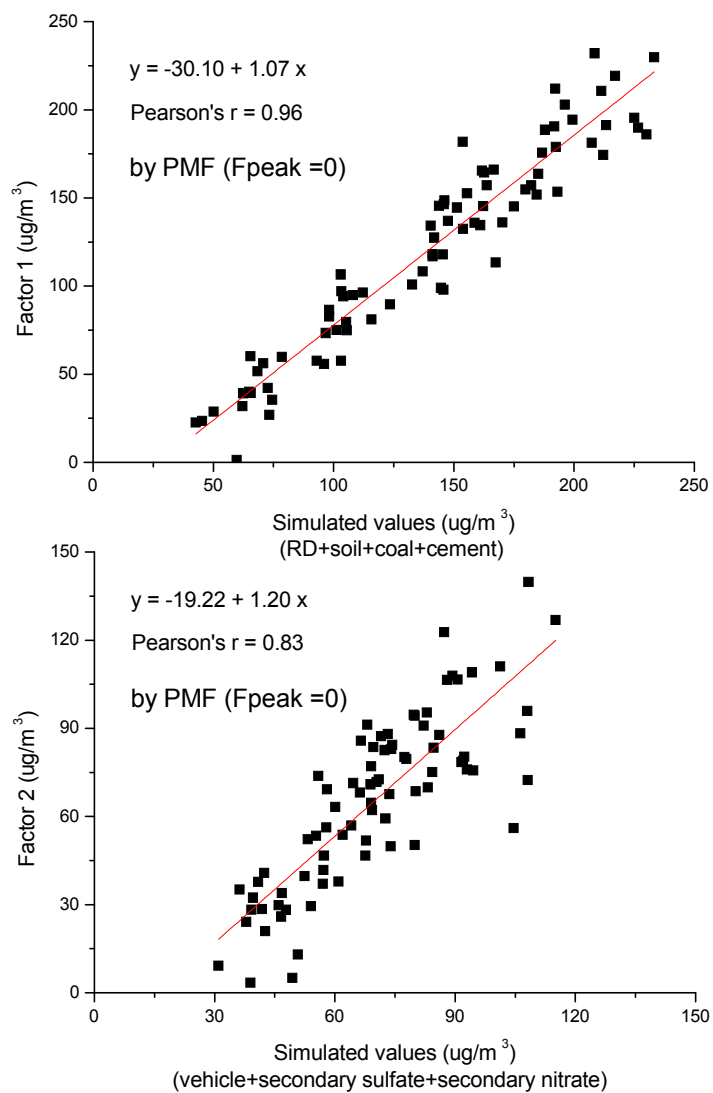


Fig. S3 The estimated contributions of factors vs. true values, by PMF ($F_{\text{peak}}=0$)

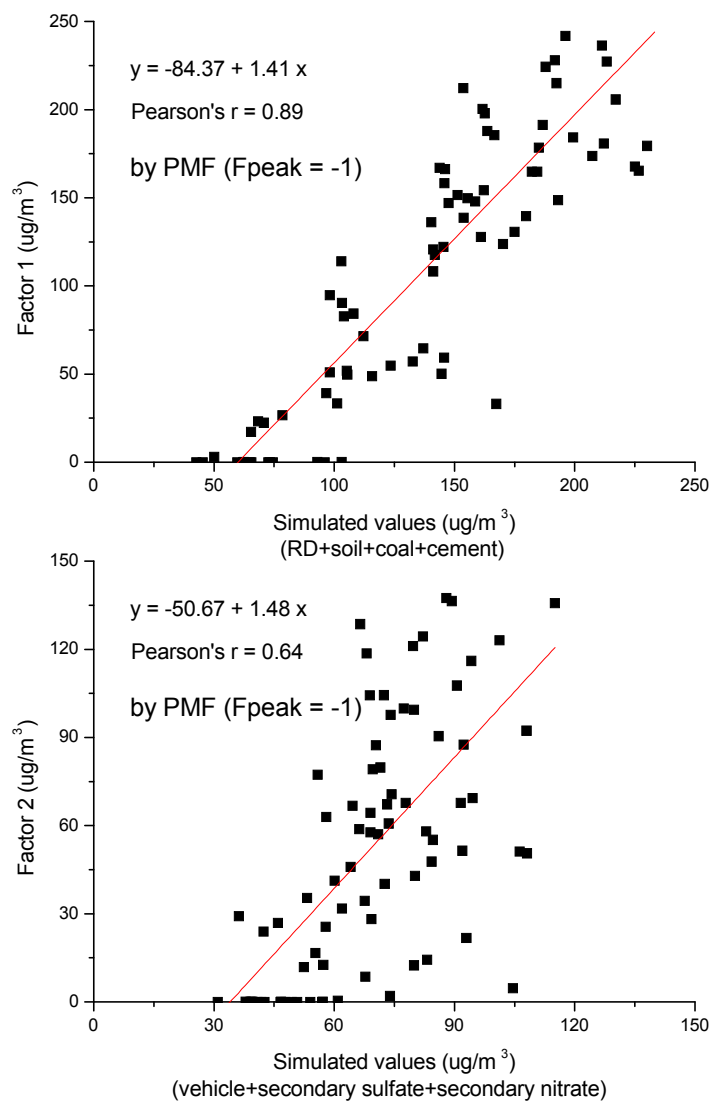


Fig. S4 The estimated contributions of factors vs. true values, by PMF (Fpeak= -1)

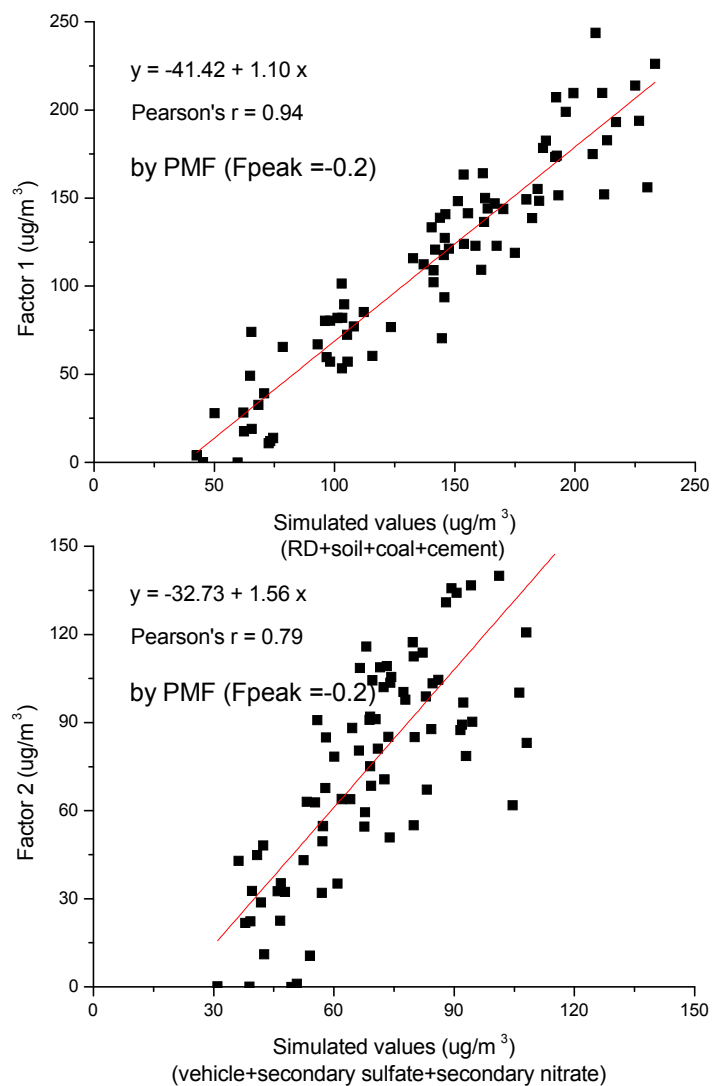


Fig. S5 The estimated contributions of factors vs. true values, by PMF ($F_{\text{peak}} = -0.2$)

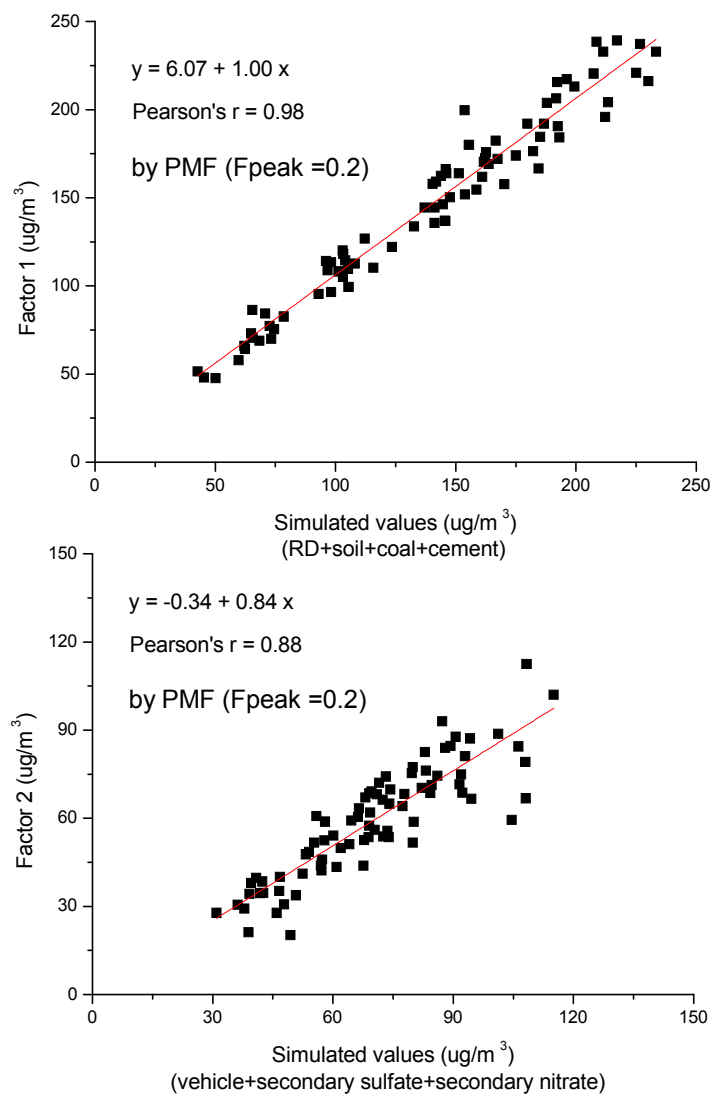


Fig. S6 The estimated contributions of factors vs. true values, by PMF ($F_{\text{peak}} = 0.2$)

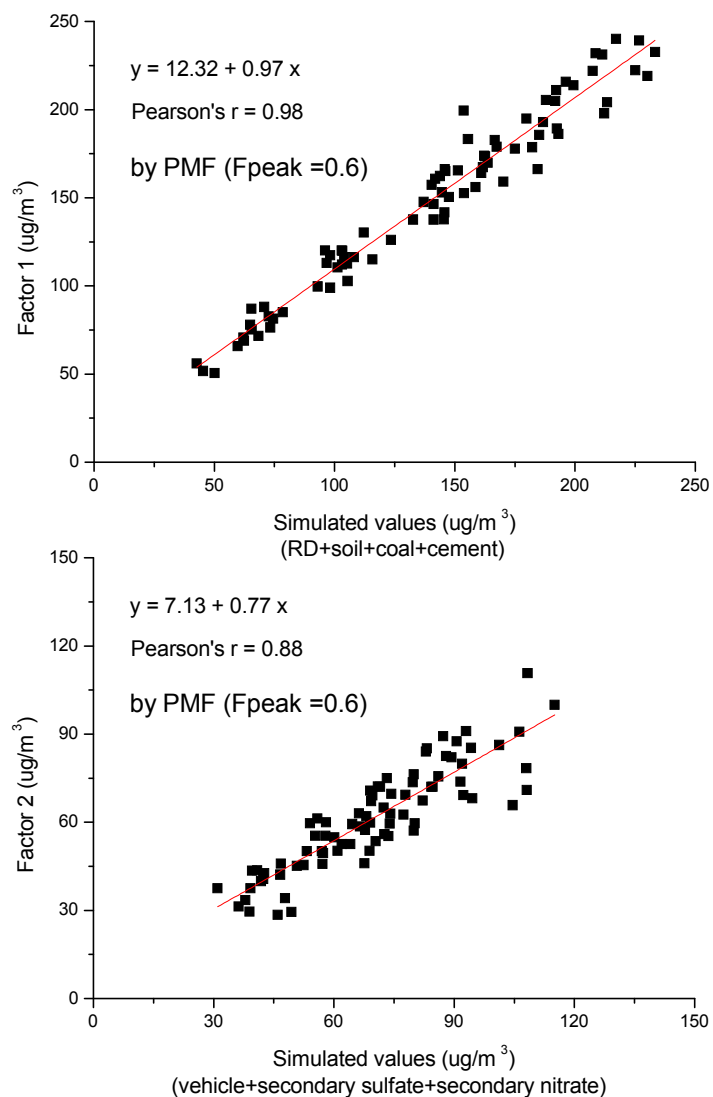


Fig. S7 The estimated contributions of factors vs. true values, by PMF ($F_{\text{peak}} = 0.6$)

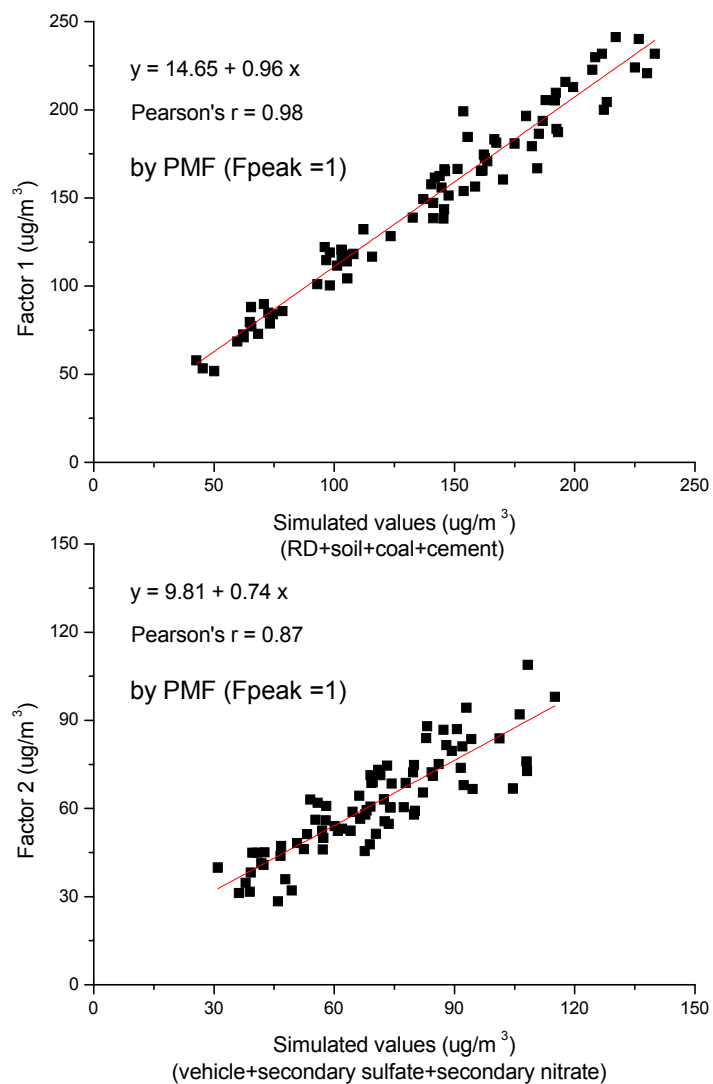


Fig. S8 The estimated contributions of factors vs. true values, by PMF ($F_{\text{peak}} = 1$)

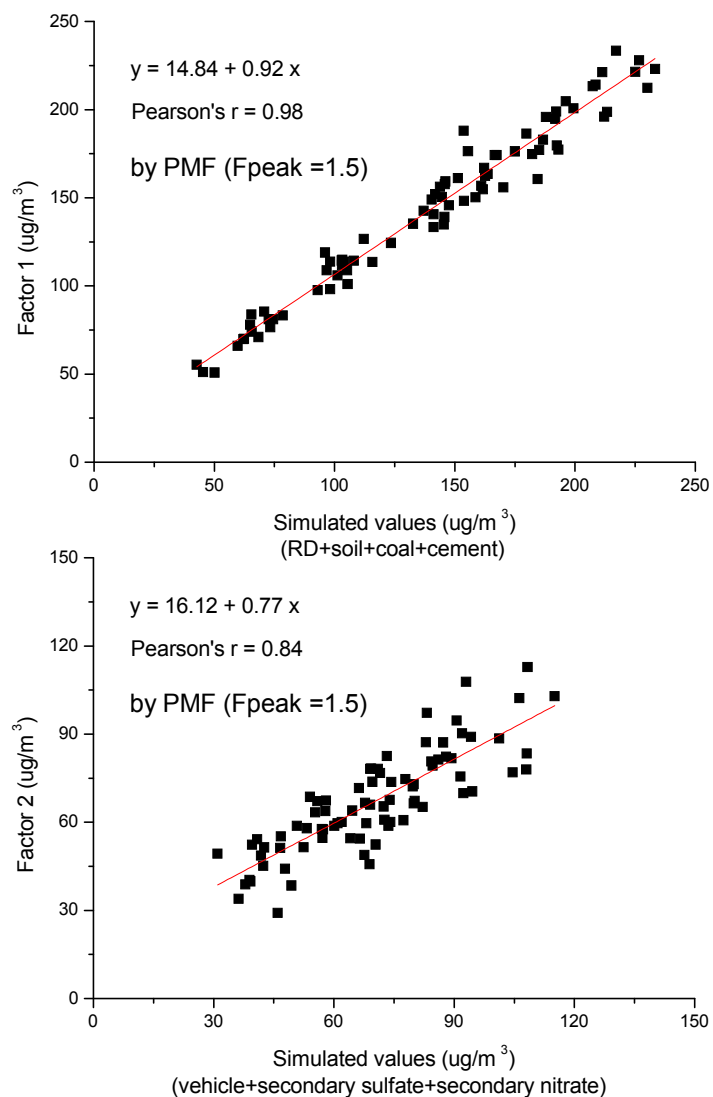


Fig. S9 The estimated contributions of factors vs. true values, by PMF (Fpeak= 1.5)

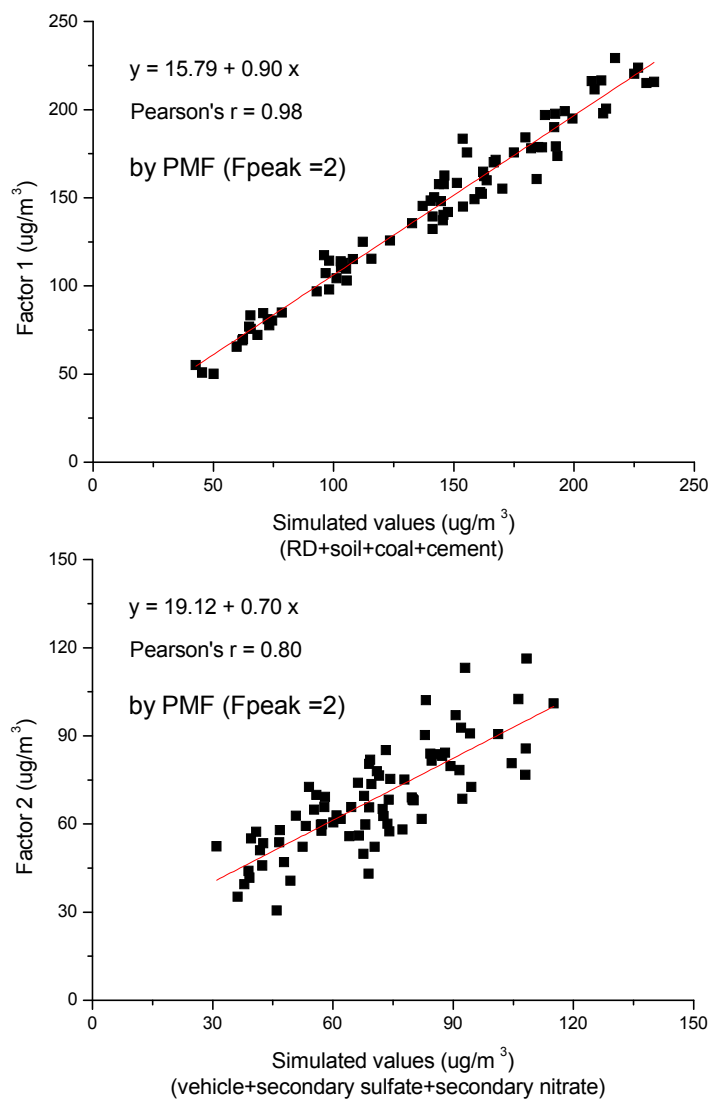


Fig. S10 The estimated contributions of factors vs. true values, by PMF (Fpeak= 2)

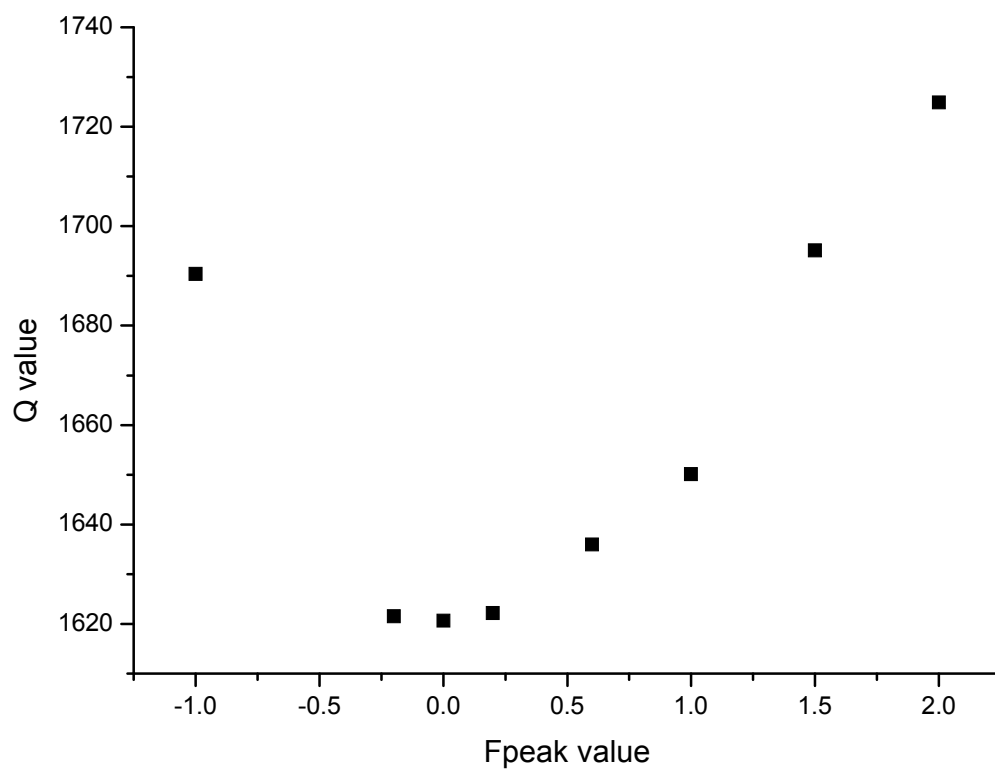


Fig. S11 the Q values for corresponding Fpeak, by PMF

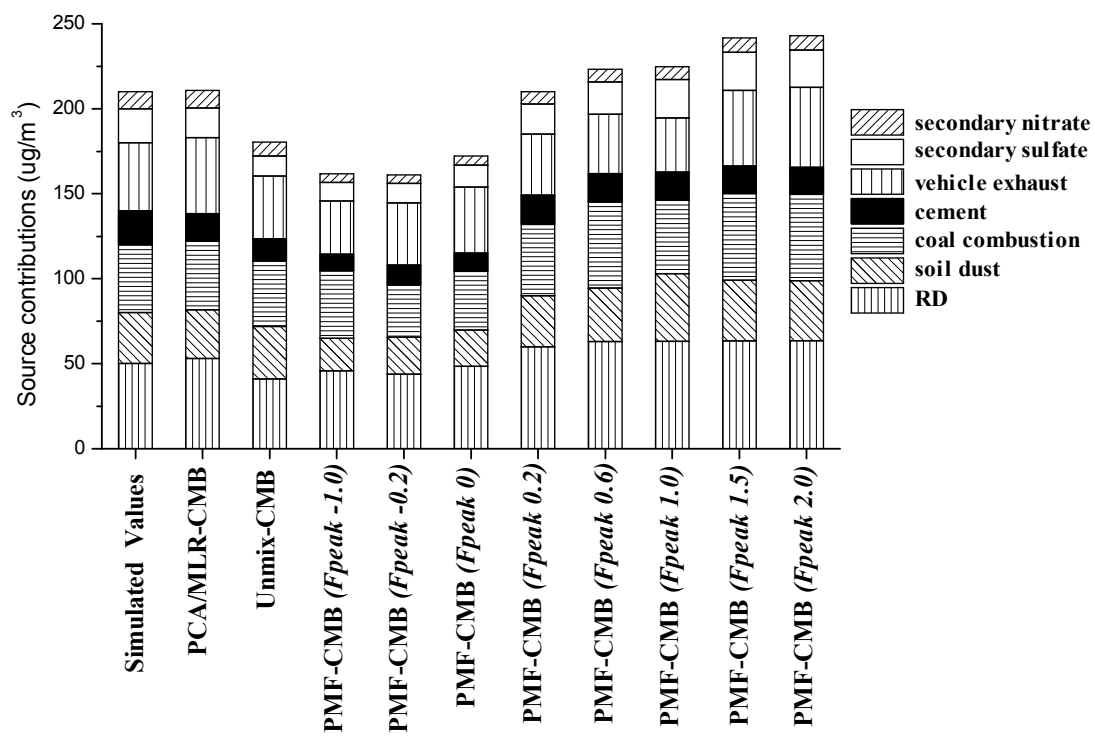


Fig. S12.

Predicted source contributions by multiply combined model, for synthetic Dataset B

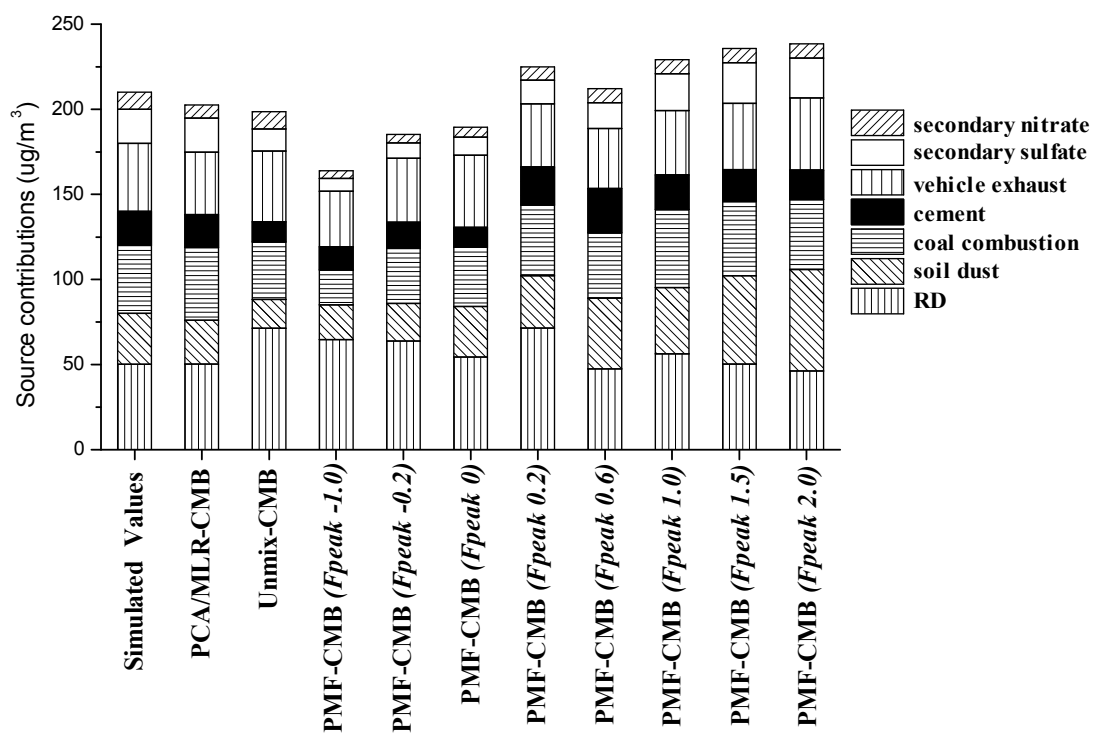


Fig. S13.

Predicted source contributions by multiply combined model, for synthetic Dataset C

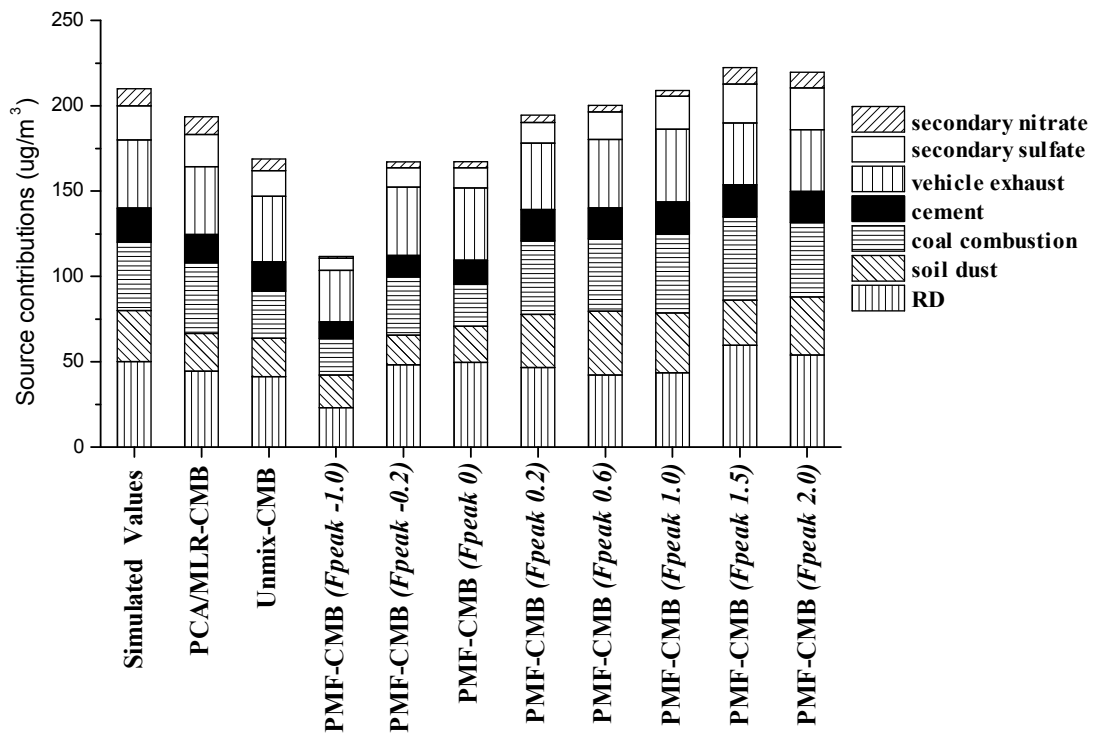


Fig. S14.

Predicted source contributions by multiply combined model, for synthetic **Dataset D**

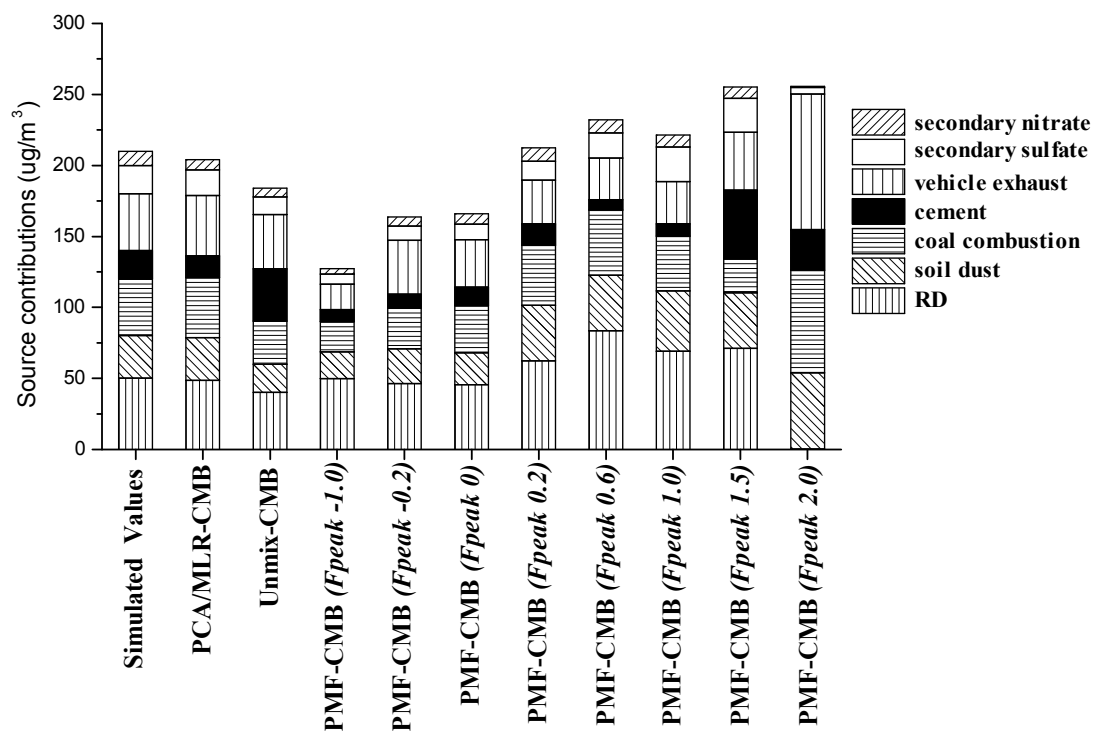


Fig. S15.

Predicted source contributions by multiply combined model, for synthetic Dataset E

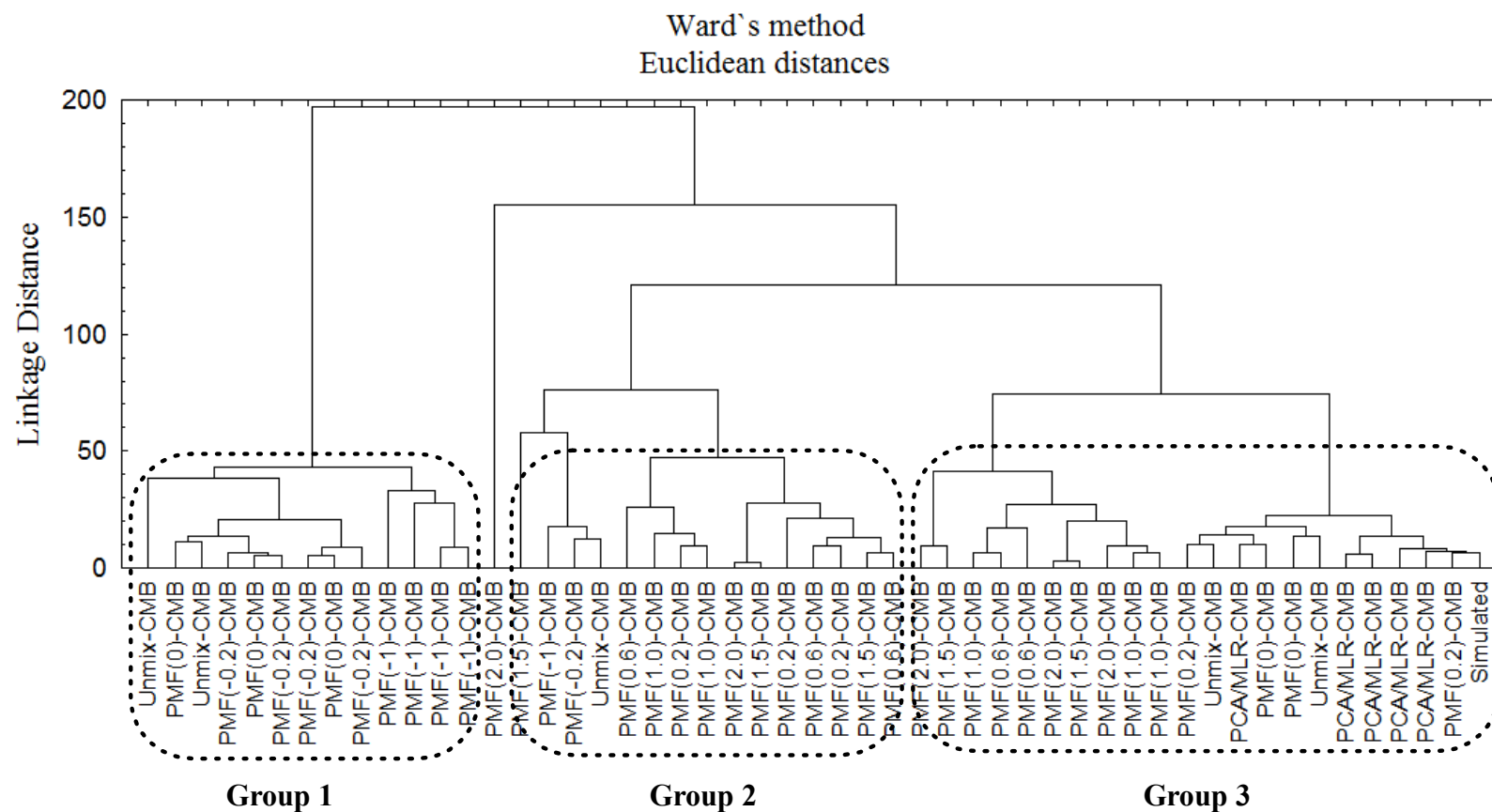


Fig. S16. Dendrogram of CA on the simulated and predicted source contributions for 50 solutions

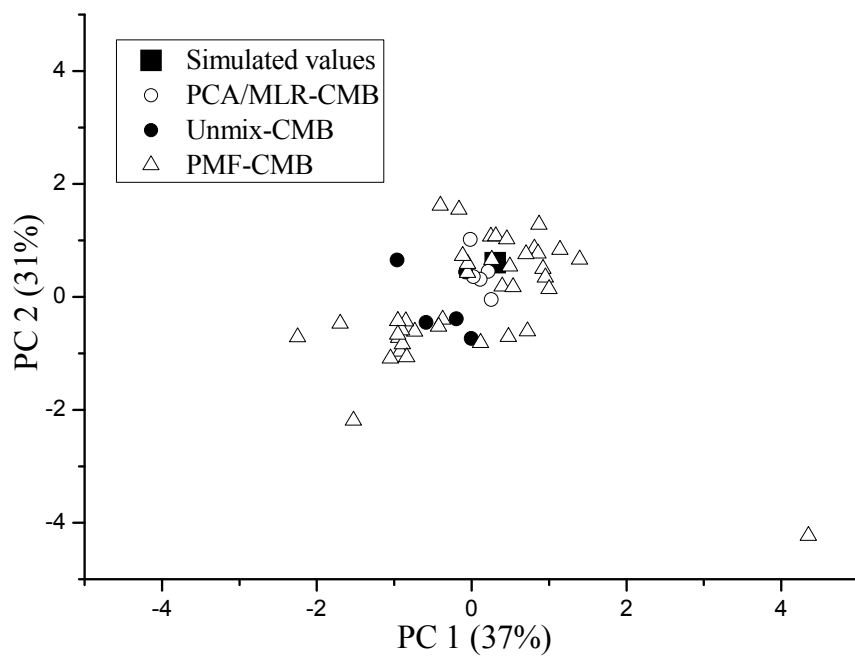


Fig. S17. Factor scores for simulated and 50 predicted contributions