

SUPPLEMENTARY MATERIAL

PM_{2.5} IN CAPE TOWN, SOUTH AFRICA: CHEMICAL CHARACTERIZATION AND SOURCE APPORTIONMENT USING DISPERSION-NORMALISED POSITIVE MATRIX FACTORIZATION

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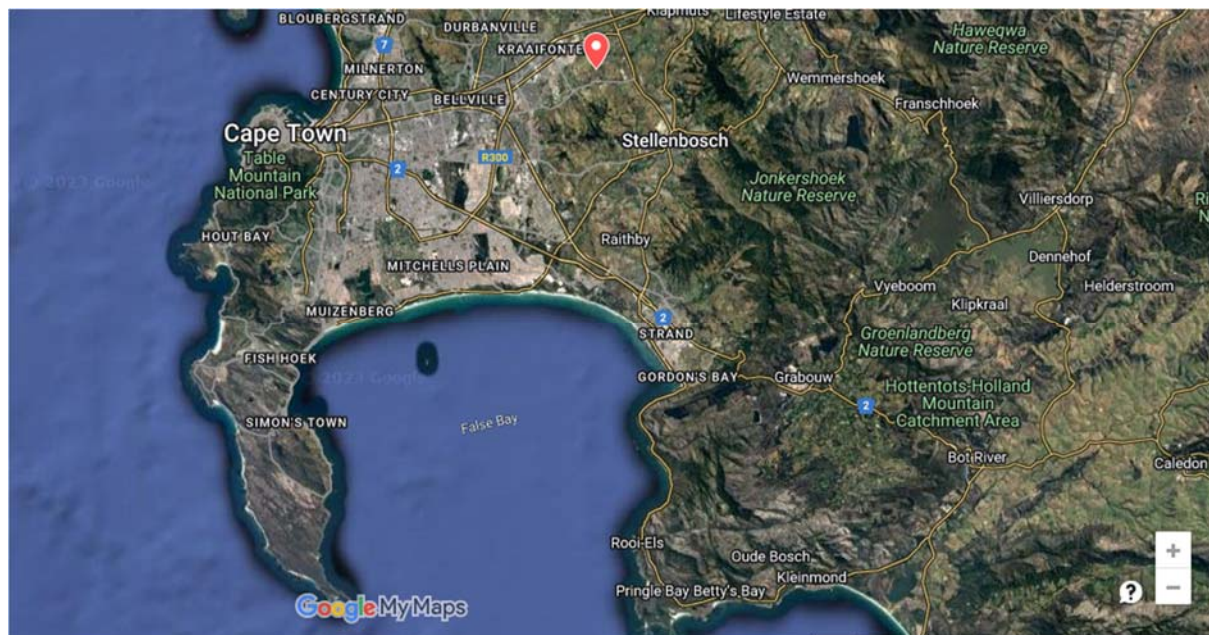


Figure S1: Kraaifontein sampling site where samples have been collected from April 2017-April 2018

Table S1: Methods and measuring equipment inventories for PM_{2.5} species in Cape Town

PM _{2.5} species	METHODS	INSTRUMENT
Total PM	Pre and post weighing (Temp:20.1-22.0; RH:43-54%)	Ultra-micro-balance (Mettler-Toledo XP6)
Soot	Diffusion system, London, UK (in batches of 20 filters)	M43D ELL Smoke Stain Reflectometer
BC	Absorption of UV light at 350 nm	Model OT21 Optical Transmissometer
UVBC	Additional absorption of UV light at 370 nm, due to organic that indicate the presence of biomass burning	Model OT21 Optical Transmissometer
Trace elements	A XEPOS 5 Energy-dispersive x-ray fluorescence (EDXRF) Spectrometer	Spectro-Analytical Instrument GmbH, Germany

Table S2: Descriptive statistics of 24-h PM_{2.5} on 121 days during April 18, 2017, to April 16, 2018, in Kraaifontein, Cape Town, South Africa

	N	Mean	Std Dev	Median	Min	Max
Full study	121	13.4	8.16	11.1	1.2	39.1
Autumn	31	11.3	5.3	10.7	1.9	21.7
Winter	30	16.1	10.4	13.2	3.2	39.1
Spring	30	17.4	8.8	18.0	1.2	32.8
Summer	30	9.1	3.7	9.3	2.0	17.3
Weekdays	83	12.0	7.2	9.9	1.2	32.8
Weekends	38	16.1	9.4	14.2	2.7	39.1

Table S3: Number of times PM_{2.5} exceeded the yearly and daily WHO air quality guidelines.

season	Daily WHO guideline (15.0 µg/m ³)	Yearly WHO guideline (5.0 µg/m ³)
Annual	38	107
Summer	1	0
Spring	17	0
Autumn	7	0
Winter	13	0

Table S4. Average PM_{2.5} concentration ($\mu\text{g}/\text{m}^3$) and meteorological data in Cape Town for each season

Seasons	PM _{2.5} ($\mu\text{g}/\text{m}^3$)	Temperature ($^{\circ}\text{C}$)	Relative Humidity (%)	Wind speed (m/s)	Rainfall (mm)
Annual	13.4	17.7	67.9	3.7	0.6
Spring	17.4	17.3	66.0	2.7	1.0
Winter	16.1	13.4	72.3	4.1	1.3
Autumn	11.3	18.8	68.5	2.8	0
Summer	9.1	21.5	64.8	5.0	0.2

Table S5: Correlation between air pollution and weather variables measured at Kraaifontein suburb in Cape Town, South Africa during 18 April 2017 and 16 April 2018.

Variables	PM _{2.5}	BC	OC	Delta-C	Temp	RH	WS
PM _{2.5}	1						
BC	0.538 0.000	1					
OC	0.554 0.000	0.986 0.000	1				
Delta-C	0.596 0.000	0.938 0.000	0.938 0.00	1			
Temp	-0.216 0.018	-0.286 0.002	-0.337 0.000	-0.306 0.001	1		
RH	-0.170 0.064	-0.087 0.343	-0.081 0.379	-0.115 0.213	-0.460 0.000	1	
WS	-0.312 0.001	-0.576 0.000	-0.593 0.000	-0.598 0.000	0.368 0.000	-0.179 0.057	1

Abbreviations: PM_{2.5}: particulate matter with an aerodynamic diameter of less than 2.5 μm , BC- Black carbon, Temp- temperature; RH- relative humidity; OC-Organic carbon; WS-wind speed

Table S6: Descriptive summaries of trace elements used in the source apportionment study of PM_{2.5} trace elemental composition measured at the Kraaifontein suburb, Cape Town during 16 April 2017 to 18 April 2018 (in µg/m³)

Elements	Detection Limit	Mean	SD	Median	Range
BC	0.07	2.367	1.460	1.990	0.000-6.589
UVBC	0.07	2.479	1.934	1.956	0.000-8.695
Si	0.1	0.515	0.506	0.381	0.020-3.021
S	0.07	1.435	0.929	1.263	0.028-4.645
Cl	0.1	0.495	0.523	0.295	0.002-2.486
K	0.07	0.244	0.226	0.167	0.004-1.527
Ca	0.11	0.301	0.218	0.252	0.029-1.147
Ti	0.05	0.036	0.029	0.032	0.004-0.158
Fe	0.05	0.182	0.153	0.141	0.005-0.778
Ni	0.05	0.010	0.006	0.011	0.002-0.025
Cu	0.05	0.009	0.009	0.006	0.002-0.048
Zn	0.05	0.046	0.049	0.028	0.002-0.302
U	-	0.003	0.002	0.002	0.000-0.009
Pb	0.05	0.004	0.004	0.002	0.002-0.031
Ba	0.05	0.011	0.007	0.007	0.004-0.033
As	0.2	0.004	0.010	0.001	0.001-0.064
Br	0.05	0.009	0.009	0.007	0.001-0.065
Se	0.05	0.003	0.003	0.002	0.000-0.021
Sb	-	0.038	0.017	0.035	0.002-0.089
V	0.05	0.010	0.028	0.001	0.001-0.162
Sr	0.05	0.009	0.002	0.009	0.004-0.014

Table S7: Descriptive statistics of Black carbon (BC), Chlorine (Cl), Potassium (K), Iron (Fe), Arsenic (As) and Bromine (Br) ($\mu\text{g}/\text{m}^3$) on seasons during 18 April 2017 to 16 April 2018 in Kraaifontein, Cape Town South Africa.

VARIABLE	AUTUMN	WINTER	SPRING	SUMMER
BC	2.811 \pm 1.240	3.552 \pm 1.586	1.676 \pm 1.090	1.414 \pm 0.650
Cl	0.325 \pm 0.345	0.331 \pm 0.422	0.520 \pm 0.496	0.808 \pm 0.650
K	0.235 \pm 0.169	0.415 \pm 0.339	0.168 \pm 0.115	0.160 \pm 0.095
Fe	0.226 \pm 0.170	0.269 \pm 0.192	0.135 \pm 0.089	0.098 \pm 0.053
As	0.002 \pm 0.002	0.014 \pm 0.016	0.001 \pm 0.002	0.001 \pm 0.000
Br	0.001 \pm 0.001	0.015 \pm 0.013	0.006 \pm 0.004	0.006 \pm 0.004

Table S8: Descriptive statistics of Chlorine (Cl) and Potassium (K) (ng/m^3) on weekends/public holidays (38 days) and weekdays (83 days) during 18 April 2017 to 16 April 2018 in Kraaifontein, Cape Town South Africa.

Variable	Mean	Std Dev	Median	Min	Max
Weekends/Public holidays					
Chlorine (Cl)	630	480	630	17	2100
Potassium (K)	350	310	240	30	1500
Weekdays					
Chlorine (Cl)	430	530	200	2	2500
Potassium (K)	200	150	150	4	710

Table S9: Descriptive statistics of 24-hour Iron levels (Fe)(ng/m^3) on 121 days during 18 April 2017 to 16 April 2018 in Kraaifontein, Cape Town, South Africa by day of the week

Variable	Mean	Std Dev	Median	Min	Max
Monday	260	230	170	20	800
Tuesday	200	150	160	40	600
Wednesday	170	100	150	5	460
Thursday	180	140	140	30	570
Friday	240	160	200	90	680
Saturday	110	80	10	10	360
Sunday	110	90	110	11	420

Table S10. PMF Input Data Statistics

Species	Category	S/N	Min	25th	Median	75th	Max	% Modeled Samples	% Raw Samples
PM2.5	Weak	0	0.687540315	4.498855017	7.19002104	11.45611676	21.58209851	82.64 %	100.00 %
BC	Strong	4.624331967	0.234974732	0.925333843	1.531306684	2.096471192	6.443454573	82.64 %	99.17 %
UV-PM	Bad	4.514638073	0.228963807	0.946964212	1.335374912	2.086744422	7.752644706	0.00 %	99.17 %
DC	Weak	0.019757171	0.00659772	0.16168474	0.16168474	0.16168474	1.852691452	35.54 %	38.84 %
Si	Strong	8.842185587	0.009058755	0.104174505	0.248413147	0.451796959	2.480326773	82.64 %	100.00 %
S	Strong	8.376147615	0.081469907	0.386863127	0.929608383	1.756662058	4.038846657	82.64 %	100.00 %
Cl	Strong	7.120149926	0.000279596	0.035259779	0.164789154	0.717378656	2.46804836	82.64 %	100.00 %
K	Strong	9.435796851	0.014790141	0.074340303	0.135804485	0.248647828	0.558780987	82.64 %	100.00 %
Ca	Strong	8.379290134	0.014639719	0.072498989	0.179832358	0.317875238	1.57589139	82.64 %	100.00 %
Ti	Strong	9.248179259	0.000700662	0.010127073	0.017964183	0.034124111	0.140554508	82.64 %	100.00 %
V	Weak	3.555549333	7.07795E-05	0.000556877	0.001111671	0.001895653	0.243657829	82.64 %	100.00 %
Fe	Strong	9.8316262	0.009644731	0.061341073	0.100670897	0.159826569	0.352872843	82.64 %	100.00 %
Ni	Strong	8.877248112	0.000170164	0.002674531	0.005902722	0.014008785	0.047166426	82.64 %	100.00 %
Cu	Weak	7.868741819	0.000393992	0.002133058	0.004397683	0.008928305	0.036073918	82.64 %	100.00 %
Zn	Strong	9.114284732	0.001881226	0.008641248	0.023628386	0.050141577	0.143640885	82.64 %	100.00 %
As	Weak	3.240283461	0.00014895	0.00047399	0.00068968	0.00132094	0.031264884	82.64 %	100.00 %
Se	Weak	4.681034847	0.000101098	0.000643565	0.001288805	0.002572683	0.009517277	82.64 %	100.00 %
Br	Weak	8.968856112	0.000518806	0.003052685	0.005044439	0.008583758	0.024017126	82.64 %	100.00 %
Sr	Weak	9.514340784	0.000431161	0.003378876	0.006772576	0.011355122	0.024891077	82.64 %	100.00 %
Sb	Weak	7.60687392	0.000519607	0.013420887	0.027447614	0.042566564	0.11318258	82.64 %	100.00 %
Ba	Weak	1.000949922	0.000779165	0.002350036	0.005603445	0.010698496	0.044836016	82.64 %	100.00 %
Pb	Strong	3.445047244	0.000212695	0.001157703	0.002153583	0.00305659	0.025353456	82.64 %	100.00 %
U	Bad	0.007666916	0.000161957	0.000652305	0.001298186	0.003516229	0.012762372	0.00 %	100.00 %
UMM	Weak	2.88	-0.709595387	2.118863316	4.879455876	8.5621706	20.47839332	82.64 %	100.00 %

Table S11. EPA PMF Diagnostics (DISP, BS, and BS-DISP) for the selected 7 factor solution

BS-DISP Diagnostics:

# of Cases Accepted:	93						
% of Cases Accepted:	93%						
Largest Decrease in Q:	-19.07						
%dQ:	-1.05						
# of Decreases in Q:	3						
# of Swaps in Best Fit:	0						
# of Swaps in DISP:	4						
Swaps by Factor:	1	0	1	1	1	1	1

DISP Diagnostics:

Error Code:	0						
Largest Decrease in Q:	0						
%dQ:	0						
Swaps by Factor:	0	0	0	0	0	0	0

BS Mapping:

	Base Factor 1	Base Factor 2	Base Factor 3	Base Factor 4	Base Factor 5	Base Factor 6	Unmapped
Boot Factor 1	99	1	0	0	0	0	0
Boot Factor 2	0	100	0	0	0	0	0
Boot Factor 3	0	1	99	0	0	0	0
Boot Factor 4	0	31	0	48	7	2	4
Boot Factor 5	0	0	0	0	100	0	0
Boot Factor 6	0	0	0	0	0	100	0

Table S12: Average source contribution ($\mu\text{g}/\text{m}^3$) to $\text{PM}_{2.5}$ derived from the PMF modelling

Source contribution	PM	BC	S
2-Stroke/Galvanizing	1.16	0.26	0.09
Soil	0.85	0.26	0.34
Sulphate/Marine Diesel	0.25	0.15	0.17
Traffic	1.09	0.29	0.06
Sea Salt	1.51	0.13	0.33
Heating/Biomass Burning/Cooking	2.06	0.50	0.01