

Vehicular Pollution as Primary Source of Oxidative Potential of PM_{2.5} in Bhubaneswar, a non-attainment city in eastern India

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Supplementary Information

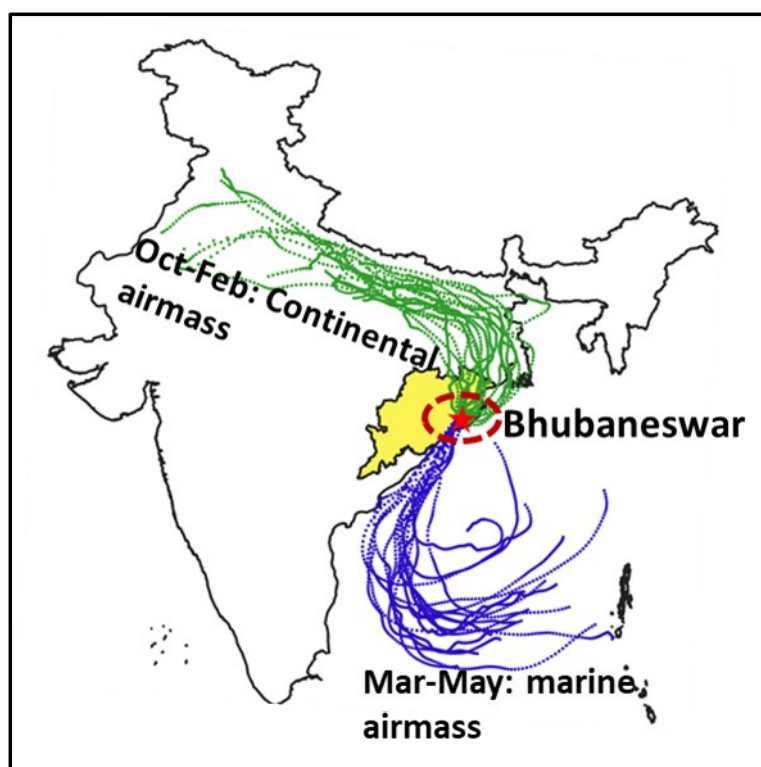


Fig. S1. Prevailing airmass during October-May at the study site during

Table T1. General meteorological characteristics during (a) MAM period (b) CAM period

Table T1 (a).

MAM	Day				Night			
Statistics	T (°C)	RH (%)	WS (km h⁻¹)	WD (degree)	T (°C)	RH (%)	WS (km h⁻¹)	WD (degree)
Mean	32.92	71.96			28.24	88.88		
Median	34.28	68.91	12.08	170	28.33	90.84	10.30	184
Standard deviation	1.88	9.31			1.32	4.41		

Table T1 (b).

CAM	Day				Night			
Statistics	T (°C)	RH (%)	WS (km h⁻¹)	WD (degree)	T (°C)	RH (%)	WS (km h⁻¹)	WD (degree)
Mean	25.59	68.57			21.18	82.84		
Median	26.83	56.74	5.4	44	20.40	87.47	0	31
Standard deviation	1.10	6.97			1.43	4.83		

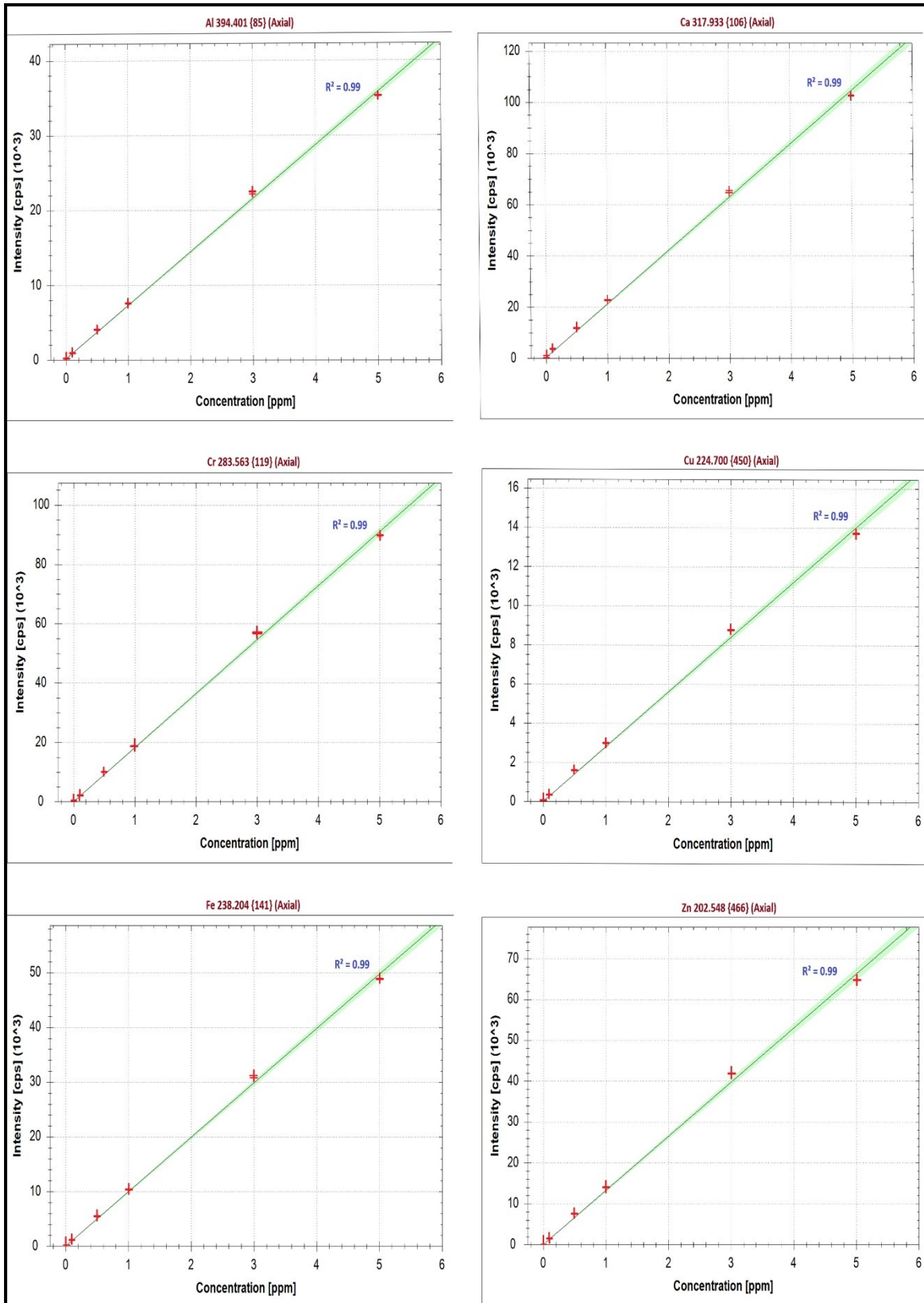


Fig. S2. Standard curve of quantification of some metals (Al, Ca, Cr, Cu, Zn, Fe) obtained from ICP-OES, iCAP 7600 Duo.

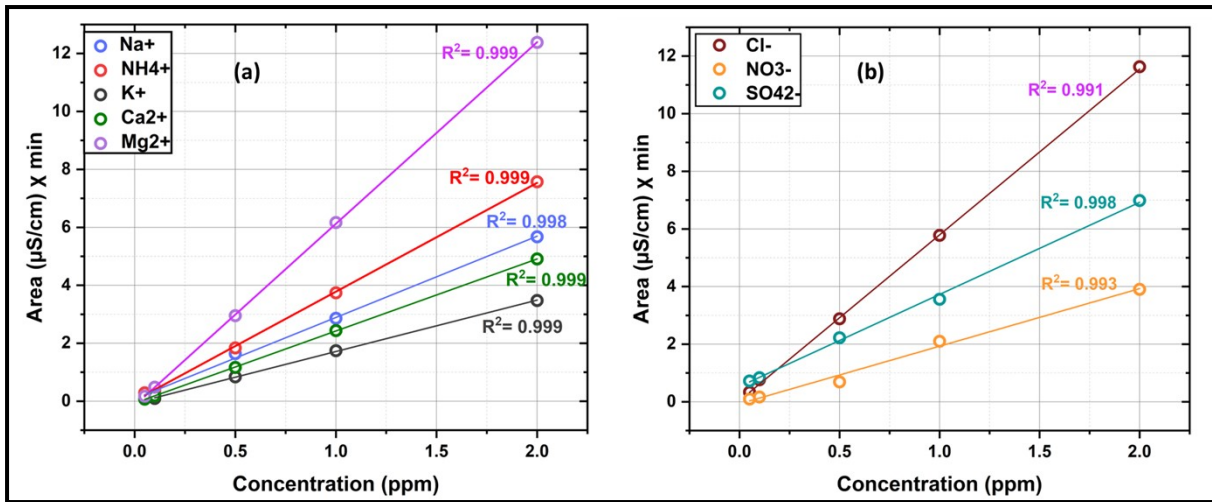


Fig. S3. Standard curve of quantification of measured (a) cations and (b) anions.

Table T2. The minimum detection limit (MDL) of blank filters based on three times the standard deviation of 10 blank filters.

Species	MDL ($\mu\text{g m}^{-3}$)
Cl ⁻	0.133
SO ₄ ²⁻	0.057
NO ₃ ⁻	0.108
NH ₄ ⁺	0.048
Ca ²⁺	0.088
Mg ²⁺	0.004
K ⁺	0.016
Na ⁺	0.030
Ba	0.007
Cr	0.018
Fe	0.019
Ni	0.013
Cu	0.024
Zn	0.019
Ca	0.003
Mn	0.007
Mg	0.01
Al	0.04
Pb	0.008
Ti	0.016
OC	0.527
EC	0.197

Text 1: To calculate ss and nss fraction of ions (Farren et al., 2019; Thakur and Thamban, 2019)

$$ssNa^+ = \frac{R_C \times Na^+ - Ca^{2+}}{R_C - R_M} \quad (1)$$

Where R_C = average ratio of Ca^{2+}/Na^+ in crust, 1.78, R_M = average ratio of Ca^{2+}/Na^+ in marine.

$$nssNa^+ = total Na^+ - ssNa^+ \quad (2)$$

$$nssK^+ = K^+ - 0.038 \times ssNa^+ \quad (3)$$

$$nssMg^{2+} = Mg^{2+} - 0.12 \times ssNa^+ \quad (4)$$

$$nssCa^{2+} = Ca^{2+} - 0.038 \times ssNa^+ \quad (5)$$

$$nssSO_4^{2-} = SO_4^{2-} - 0.25 \times ssNa^+ \quad (6)$$

Text 2

PMF considers data sets of the chemical species (in $\mu g/m^3$) as $[n \times m]$ matrix where n is the number of samples and m is the measured chemical species. The main goal of the model is to determine the number of factors (p), source profile (f) of each source and the relative contribution g by each factor to each measured sample as given in equation 7.

$$x_{ij} = \sum_{k=1}^p g_{ik} f_{kj} + e_{ij} \quad (7)$$

where x_{ij} is the concentrations of species j measured on sample i , p is the number of factors, g_{ik} is the relative contribution of factor k to sample i , f_{kj} is the concentration of species j in the emission profile of factor k , and e_{ij} is the residuals in the PMF result for species j on sample i .

The main objective is to find the best combination of g_{ik} and f_{kj} to reproduce x_{ij} . The values of f_{kj} and g_{ik} were determined by minimizing Q for a given factor number p , and Q can be defined as follows.

$$Q = \sum_{j=1}^m \sum_{i=1}^n \frac{e_{ij}^2}{s_{ij}^2} \quad (8)$$

here s_{ij} is the uncertainty of species j on sample i .

The uncertainty, s_{ij} can be calculated as follows:

$$s_{ij} = \sqrt{(\text{Error fraction} \times \text{Concentration})^2 + (\text{MDL})^2} \quad (9)$$

where MDL is the minimum detection limit enlisted in **Table T2** and error fraction is the measure of the standard deviation of the species divided by the square root of the total number of analyzed species.

A complete description of the algorithm and mathematical equation is available elsewhere (Norris et al., 2014; Paatero, 1997; Paatero and Tapper, 1994).

Table T3. S/N ratio of different species and their categorization in both the PMF run

Species	PMF-1 during MAM period		PMF-2 during CAM period	
	S/N	Category	S/N	Category
Al	0.5	Weak	1.4	Strong
Mg	6.5	Strong	7.0	Strong
Ca	8.9	Strong	9.0	Strong
Cu	8.6	Strong	8.8	Strong
Cr	0.7	Weak	2.6	Strong
Mn	0.1	Bad	1.2	Strong
Fe	6.6	Strong	7.6	Strong
Ni	0.0	Bad	0.0	Bad
Ti	0.0	Bad	0.2	Bad
Zn	2.5	Strong	4.2	Strong
Pb	0.0	Bad	0.0	Bad

Ba	0.0	Bad	0.1	Bad
Na ⁺	8.7	Strong	8.4	Strong
NH ₄ ⁺	8.9	Strong	9.0	Strong
K ⁺	8.6	Strong	8.8	Strong
Ca ²⁺	6.5	Strong	5.9	Strong
Mg ²⁺	9.0	Strong	8.9	Strong
Cl ⁻	4.6	Strong	4.4	Strong
NO ₃ ⁻	5.6	Strong	8.2	Strong
SO ₄ ²⁻	9.0	Strong	9.0	Strong
OC	7.8	Strong	8.5	Strong
EC	7.7	Strong	8.3	Strong

Table T4. Summary of PMF and error estimation diagnostics by PMF run during MAM period (The red highlighted portion shows the factor considered in the study).

Diagnostic	5 factors	6 factors	7 factors
Q _{true} /Q _{expected}	6.5	5.9	5.1
DISP %dQ	< 0.1%	< 0.1%	< 0.1%
BS mapping < 100%	88	100	72
BS-DISP % swaps	0	0	67

Table T5. Summary of PMF and error estimation diagnostics by PMF run during CAM period. (The red highlighted portion shows the factor considered in the study).

Diagnostic	4 factors	5 factors	6 factors
Q _{true} /Q _{expected}	9.4	7.3	6.5
DISP %dQ	< 0.1%	< 0.1%	< 0.1%

BS mapping < 100%	91	100	100
BS-DISP % swaps	0	0	17

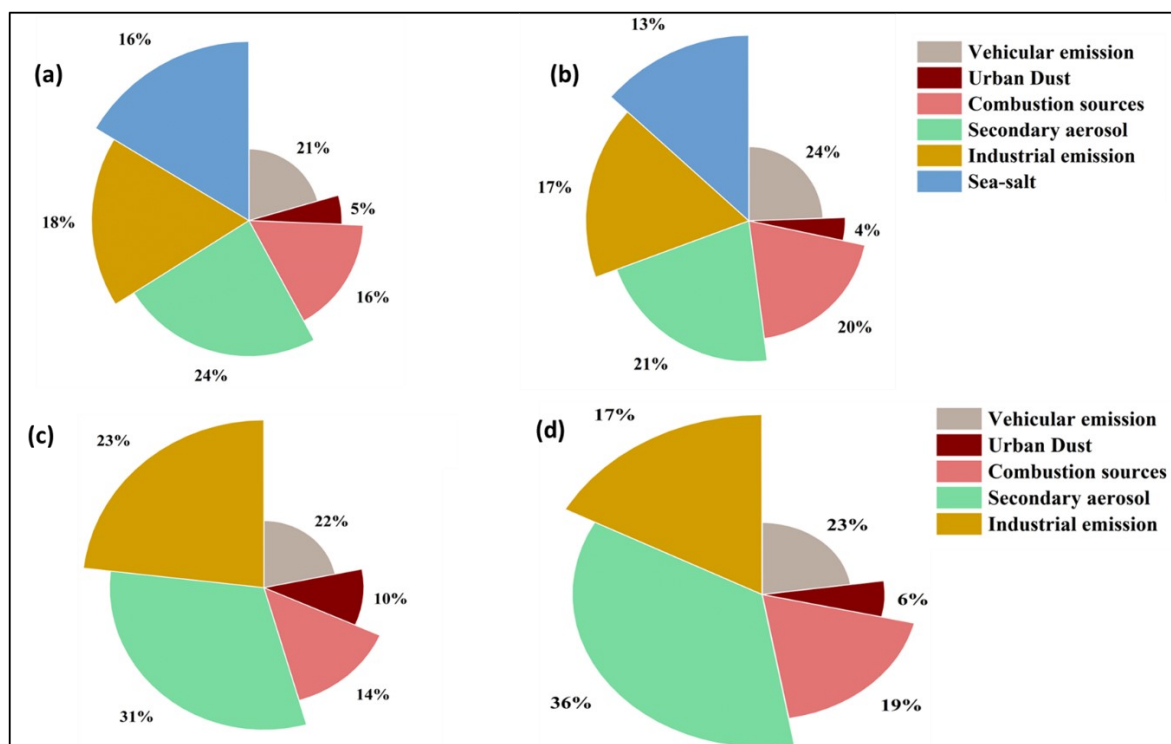


Fig. S4. Percentage contributions of different sources to PM_{2.5} mass concentration during (a) daytime (b) nighttime of MAM period (c) daytime (d) nighttime of CAM period

Table T6. Step-wise MLR-WLS through origin between DTTv and PMF source contributions during (a) MAM and (b) CAM periods.

Table T6 (a)

Model	Model	Unstandardized Coefficients	Standardized	t-stat	p-
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No.		(nmol.min ⁻¹ .μg source ⁻¹)		Coefficients		value
		B	Standard Error	Beta		
1.	Secondary aerosol	0.573	0.046	0.798	12.542	0.000
2.	Secondary aerosol	0.366	0.056	0.509	6.549	0.000
	Industrial emission	0.263	0.049	0.414	5.333	0.000
3.	Secondary aerosol	0.259	0.054	0.360	4.828	0.000
	Industrial emission	0.235	0.044	0.370	5.336	0.000
	Urban dust	0.225	0.044	0.309	5.078	0.000
4.	Secondary aerosol	0.179	0.057	0.249	3.169	0.002
	Industrial emission	0.203	0.043	0.320	4.745	0.000
	Urban dust	0.195	0.043	0.268	4.536	0.000
	Combustion sources	0.185	0.057	0.234	3.262	0.002
5.	Secondary aerosol	0.111	0.055	0.154	1.999	0.039
	Industrial emission	0.104	0.040	0.203	4.289	0.000
	Urban dust	0.131	0.043	0.180	3.034	0.003
	Combustion sources	0.209	0.053	0.264	3.941	0.000
	Vehicular emission	0.282	0.053	0.317	3.892	0.000

Table T6 (b).

Model No.	Model	Unstandardized Coefficients (nmol.min ⁻¹ .μg source ⁻¹)		Standardized Coefficients	t-stat	p-value
		B	Standard Error	Beta		
1.	Vehicular emission	1.548	0.070	0.886	21.965	0.000
2.	Vehicular emission	1.000	0.095	0.573	10.573	0.000
	Combustion sources	0.850	0.114	0.403	7.434	0.000

3.	Vehicular emission	0.765	0.096	0.438	7.969	0.000
	Combustion sources	0.698	0.107	0.330	6.503	0.000
	Secondary aerosol	0.395	0.072	0.259	5.463	0.000
4.	Vehicular emission	0.678	0.092	0.388	7.342	0.000
	Combustion sources	0.551	0.106	0.261	5.181	0.000
	Secondary aerosol	0.369	0.068	0.242	5.417	0.000
	Industrial emission	0.375	0.087	0.177	4.305	0.000
5.	Vehicular emission	0.687	0.091	0.393	7.559	0.000
	Combustion sources	0.452	0.113	0.214	4.001	0.000
	Secondary aerosol	0.364	0.067	0.238	5.426	0.000
	Industrial emission	0.339	0.087	0.160	3.895	0.000
	Urban dust	0.101	0.044	0.088	2.317	0.022

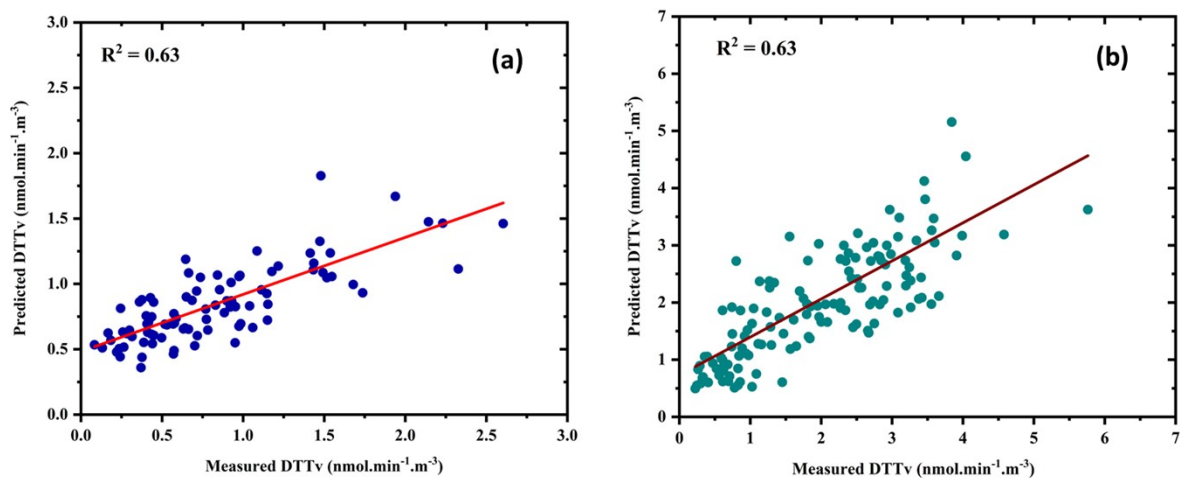


Fig. S5. Linear regression between measured DTTv and predicted DTTv during (a) MAM (b) CAM periods.