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Environmental Chemistry

Supplementary Material

Seasonal variations in characteristics, sources and diurnal patterns of carbonaceous and water-soluble constituents in urban aerosols from east coast of tropical India

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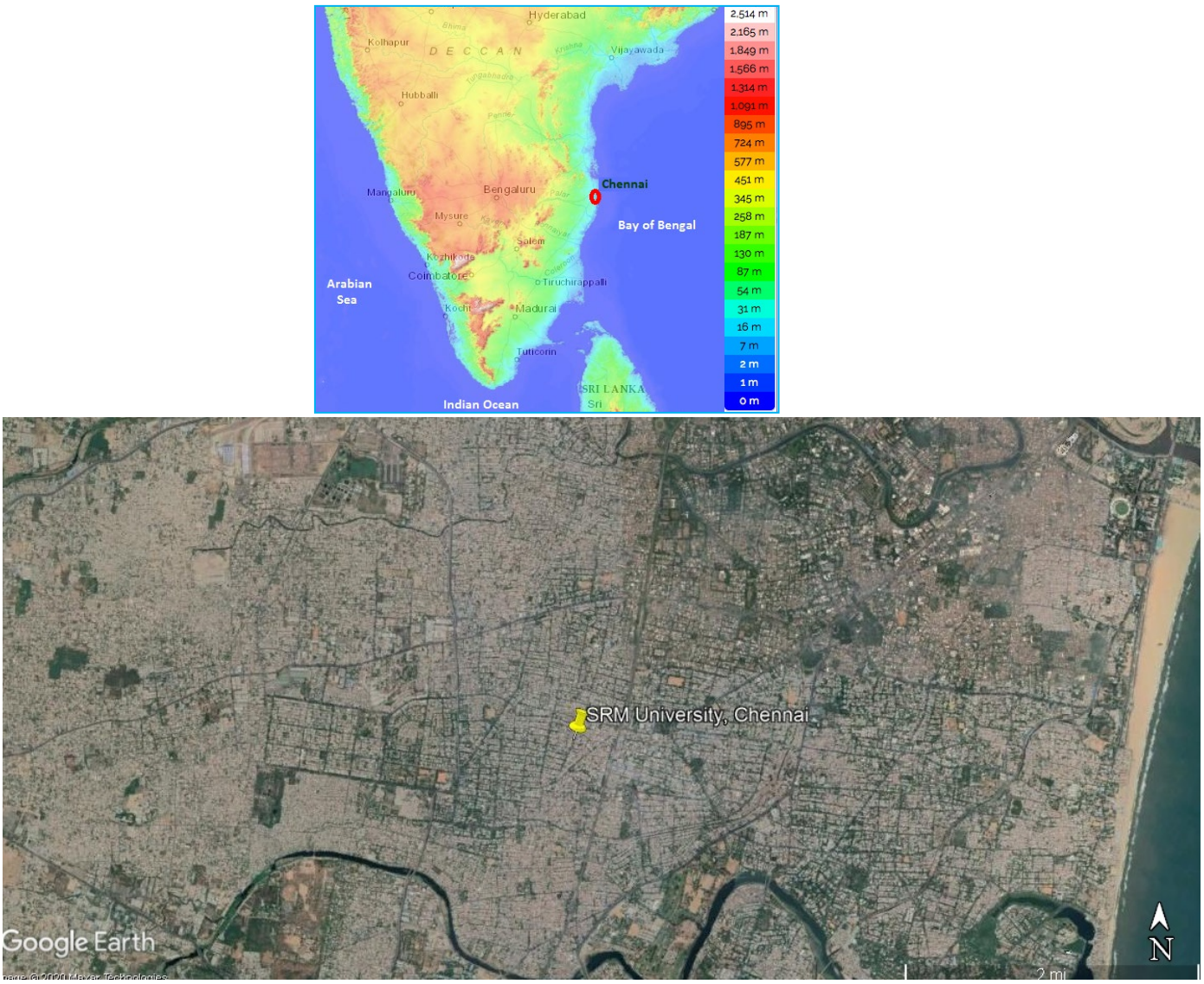

Figure S1. Geographical location (indicated by red circle) of Chennai city along the south-west of tropical peninsular India. The color scale indicates the topographic height. (Source: www.mapsofindia.com). The location of the sampling site, SRM University (indicated by yellow pin), in Chennai was shown as google map in the bottom image.

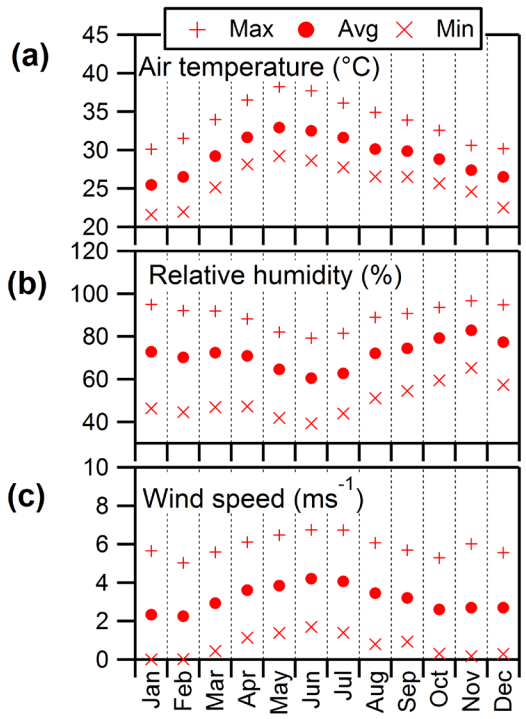

Figure S2. Monthly average values of meteorological parameters over the sampling site in Chennai during 2017-2018.

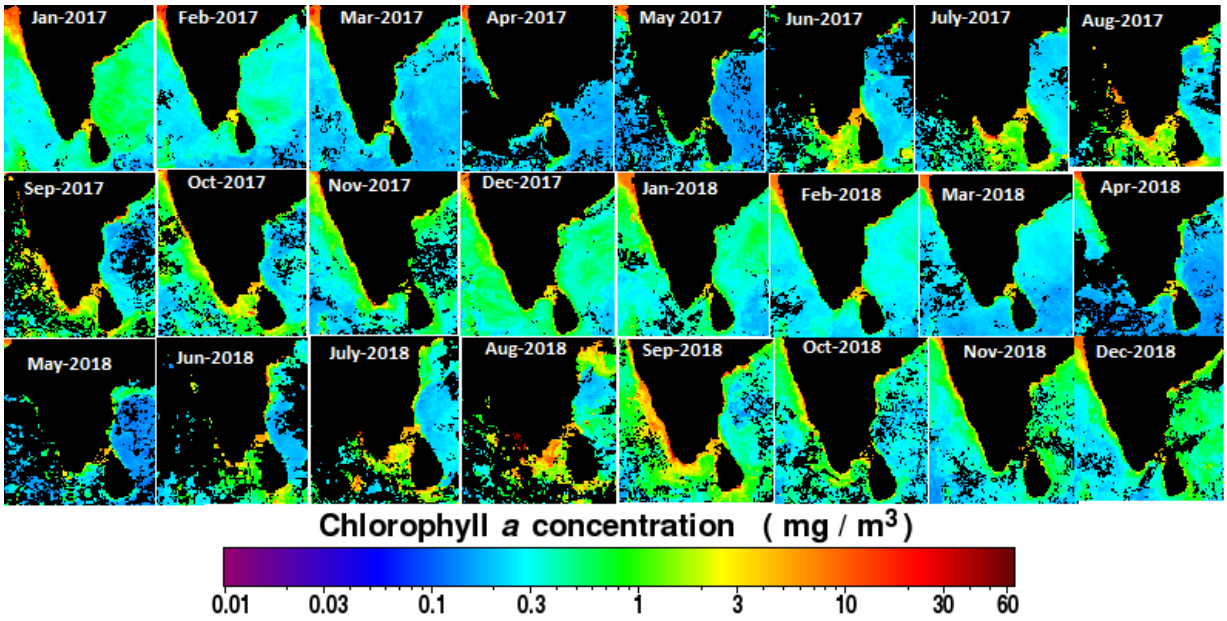

Figure S3. Monthly variations in Chlorophyll a concentrations over the tropical peninsular India during 2017-2018, Source: https://oceancolor.gsfc.nasa.gov/

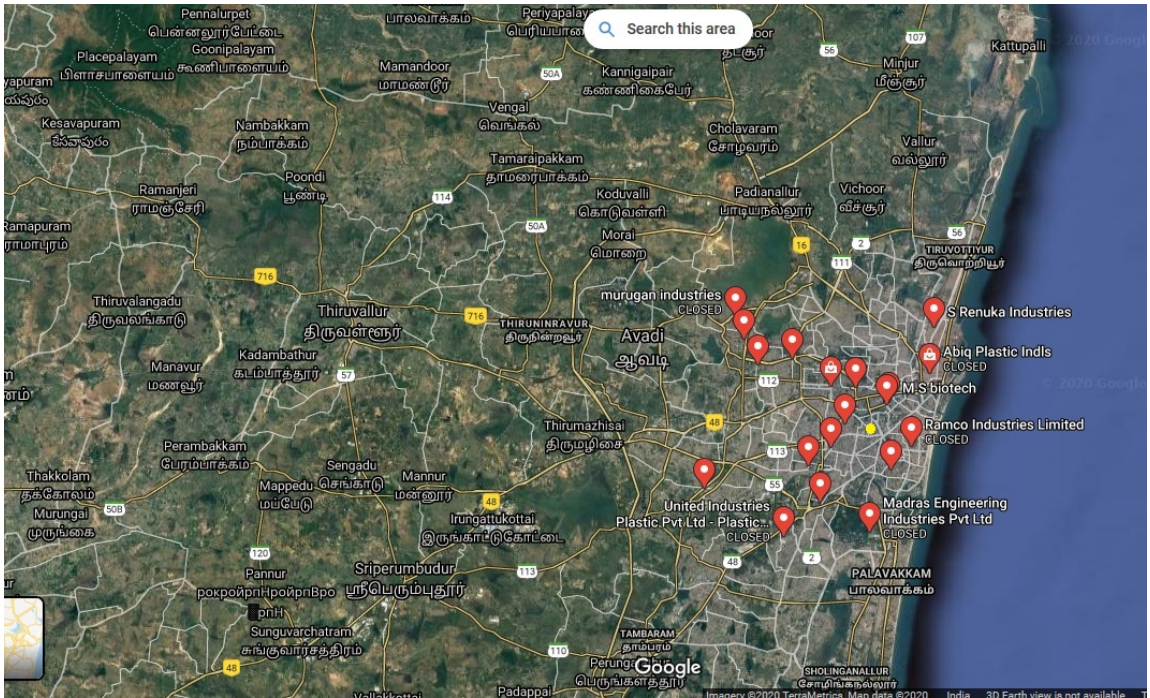

Figure S4. Google map, showing the sampling site (indicated by yellow circle) surrounded by the major industries as well as quarries indicated by red colored markers in the Chennai city.

Text S1

The aim of this model is to identify the number of factors p, the species profile f of each source and the relative contribution g by each factor to each measured sample as given below.

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

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.

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

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

The uncertainty of the PMF solution is calculated using displacement (DISP) analysis and bootstrapping (BS) analysis. DISP analysis revealed that each fitted element of the factor profile in the solution is "displaced" by predetermined error levels to determine changes, or swaps, in the factor profiles. We found that no swaps were occurred at the lowest level. With BS, various PMF solutions are generated by using a series of data sets that are resampled versions of the original data set. Each BS factor is mapped to a base factor of the original PMF solution as confirmed by comparing the factor contributions. The threshold of the minimum correlation for mapping was 0.6, and 70 bootstrapping runs were carried out. All BS factors could be mapped, and only BS Factor 7 showed mapping to the base Factor below 100% (about 99%) as given below in Table S6.

Text S2: Quality assurance

All potential precautions were taken carefully to minimize the contaminations during the sampling collection, storage and chemical analysis. PM_{10} was measured gravimetrically using a pre-calibrated digital microbalance (Satorius, LA 130 S–F). Filter samples were weighed thrice before and after the sample collection and error was less than 10% on average. In order to remove the moisture (in case) in the filter samples, all aerosol sampled filters are desiccated irrespective of the relative humidity. Moisture content in the filters was removed by keeping them in a desiccator containing silica gel crystals at room temperature for 2-4 hours before weighing the final mass, since quartz fiber filters (QFF) are very sensitive to humidity (moisture) conditions. To avoid the flake off of the filter fibers after the collection, filter samples were stored in a pre-baked (450ºC for 4-6 hours) glass bottles with Teflon lined screw caps and stored at -20 ºC until the analysis of chemical composition.

Table S1: Summary of key diagnostic results of the PMF analysis having seven-factor solution in the PMF calculation. Q is a PMF quality-of-fit parameter, Q_{robust} indicates Q excluding points which did not fit. $Q_{expected}$ is the calculated Q, whereas %dQ indicates percent change in Q when swaps occur.

Diagnostic	7- factor solution
$Q_{robust/Qexpected}$	3.78
DISP %dQ	<0.1%
Number of DISP swaps	0
Factors with BS (80 runs) < 100%	Factor 7 (98.75%)
BS unmapped	0