Supplement of Atmos. Chem. Phys., 21, 8761–8773, 2021
https://doi.org/10.5194/acp-21-8761-2021-supplement

Atmospheric Chemistry and Physics
Open Access

Supplement of

Physical and chemical properties of urban aerosols in São Paulo, Brazil: links between composition and size distribution of submicron particles

Djacinto Monteiro dos Santos et al.

Correspondence to: Djacinto Monteiro dos Santos (djunior@if.usp.br)

Positive Matrix Factorization Analysis

Time series of mass spectra for the organic component measured by ACSM from m/z 12 to m/z 100 was analyzed by Positive Matrix Factorization (PMF), using IGOR™-based source finder. Before analysis, the errors from incorrect and non-representative spikes were eliminated. The "weak" m/z's (signal-to-noise ratio between 0.2 and 2) were downweighted by a factor of 2, and the "bad" m/z's (signal-to-noise ratio smaller than 0.2) were removed. The analysis was run for a number of factors from 1 to 10. The identification of PMF factors was based on the correlation of their time series and mass spectra with external tracers and mass spectra from the AMS spectra database. Summary of PMF solutions are described in Table S1. The four-factor solution was chosen after carefully checking the quality of the fit parameter, mass spectra, correlation with external tracer and diurnal variability. A great reduction in the total residuals (Figure S1) is shown when going from one-factor to the four-factor solution. The rotational ambiguity of the four-factor solution was examined by varying the fpeak parameter from -1 to 1 in intervals of 0.1 (Table S1) and a little impact on the Q/Q_{exp} was observed for this parameter.

Table S1. Summary of PMF solutions.

Number of factors	Q/Q_{ext}	fpeak	Description
1-2	3.75 - 2.65		Large residuals at some time periods and m/z’s
3	2.46		Three factors linked to BBOA, OOA and HOA. Total residuals are significantly reduced, however residuals are still large at specific m/z’s, particularly m/z 43, 55, 60 and 73.
4	2.31		Optimum number of factors: Factor splitting shows a new factor linked to HOA. Residuals are significantly lower at m/z 43, 55, 60 and 73.
4	2.3105 - 2.311	-1 to 1	Little impact from *fpeak* on the Q/Q_{exp}. Factors are nearly identical for different *fpeak*.
5 - 8	2.17 - 1.85		Factor splitting appears as shown by unrealistic zeroes in factor time series with a single m/z peak in factor MS.

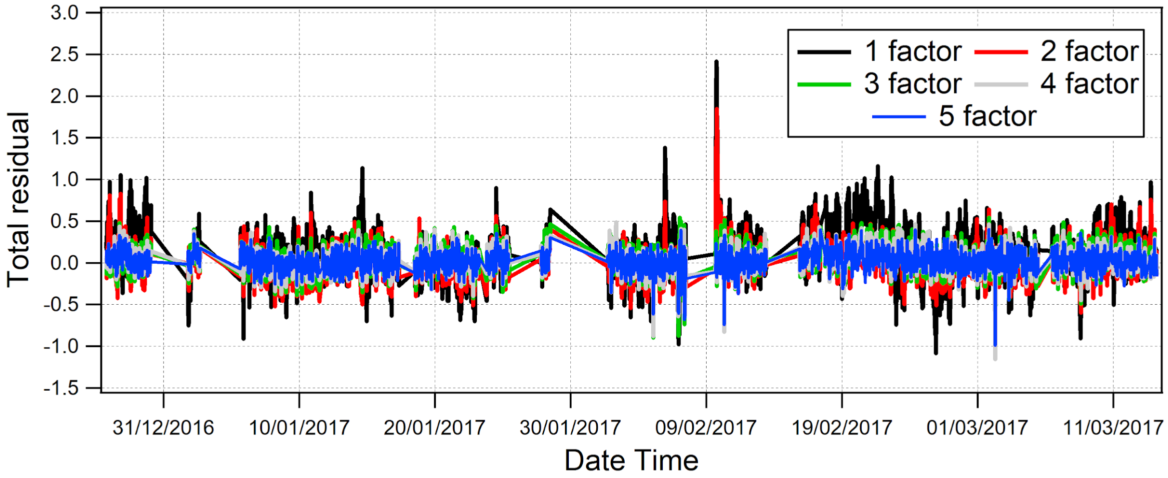

Figure S1 - Time series of total ion residuals from one factor PMF solution to five factors PMF solution.

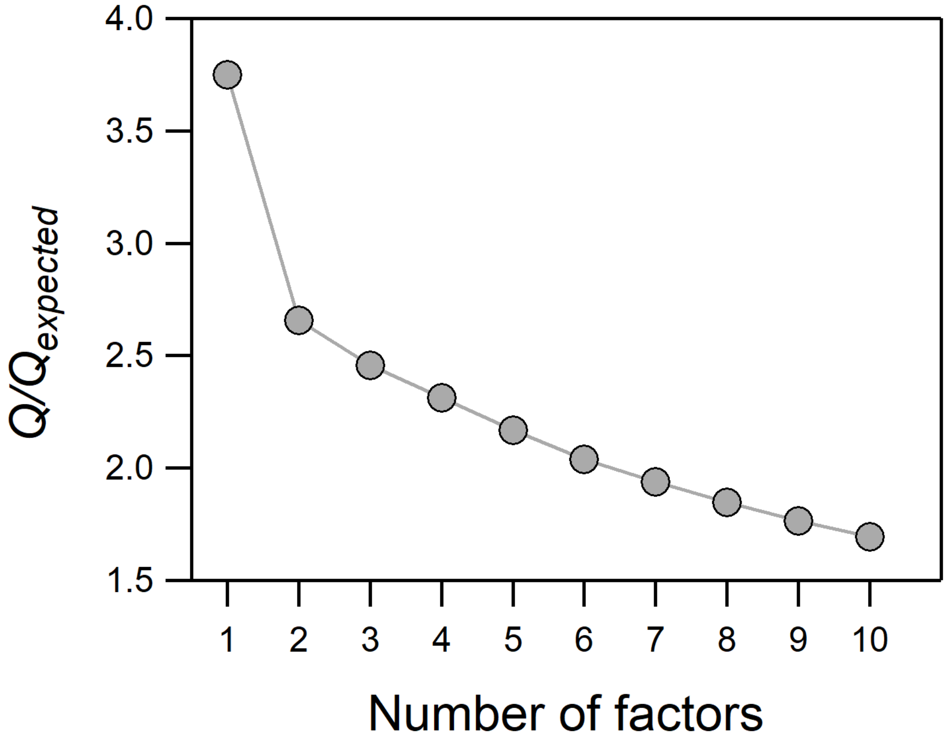

Figure S2 - Dependence of the quality-of-fit parameter Q/Qexpected on the number of factors

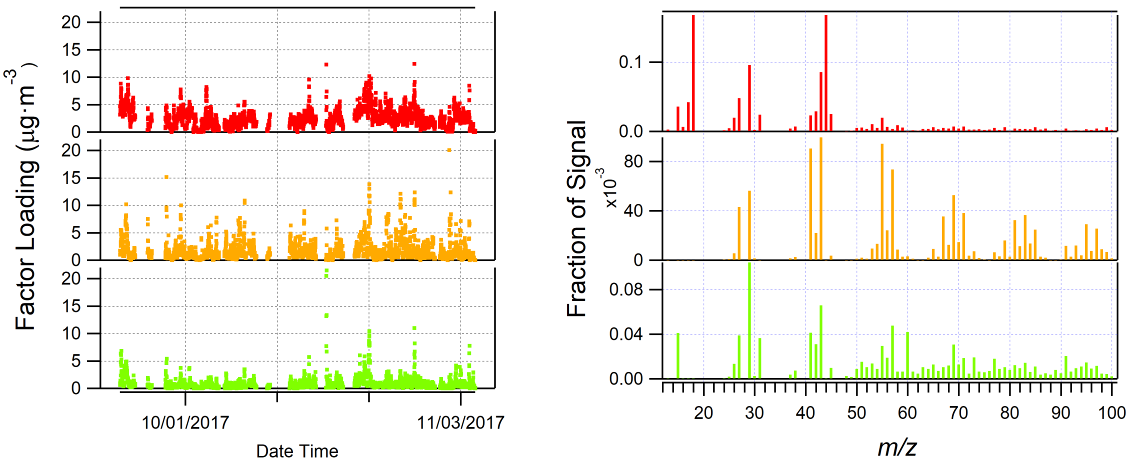
(a) (b)

Figure S3 - Results of the PMF analysis for 3 factors: (a) time series of factor loadings and (b) factor profiles.

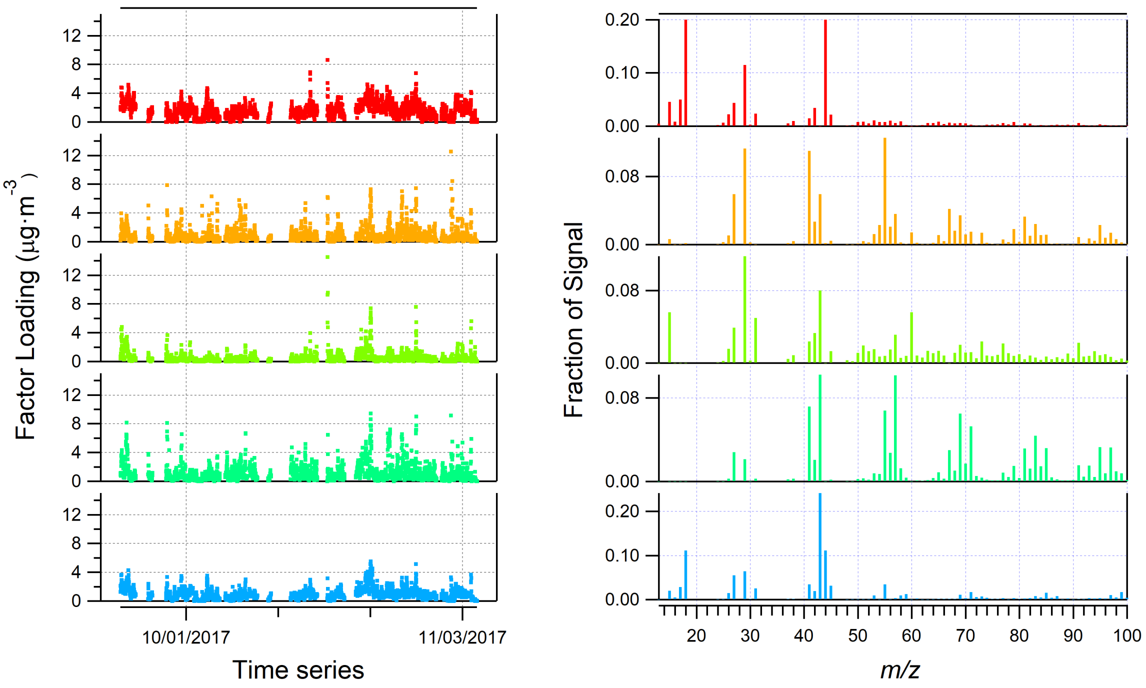
(a) (b)

Figure S4 - Results of the PMF analysis for 5 factors: (a) time series of factor loadings and (b) factor profiles.

S2. Multilinear Regression (MLR) model

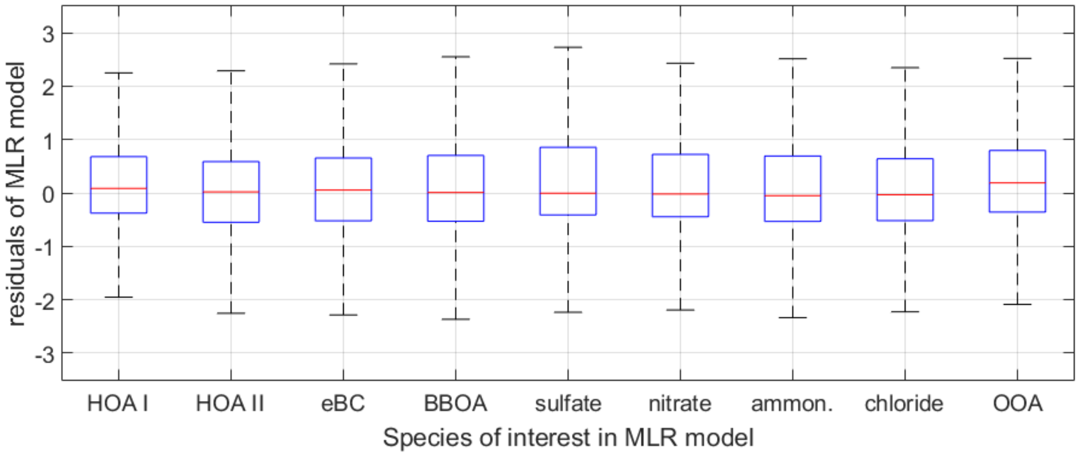

Figure S5 - Results of the MLR models: boxplot of studentized residuals for all species of interest. Time series of volume of particle size modes (i.e., nucleation, Aitken and accumulation) were used as predictors.

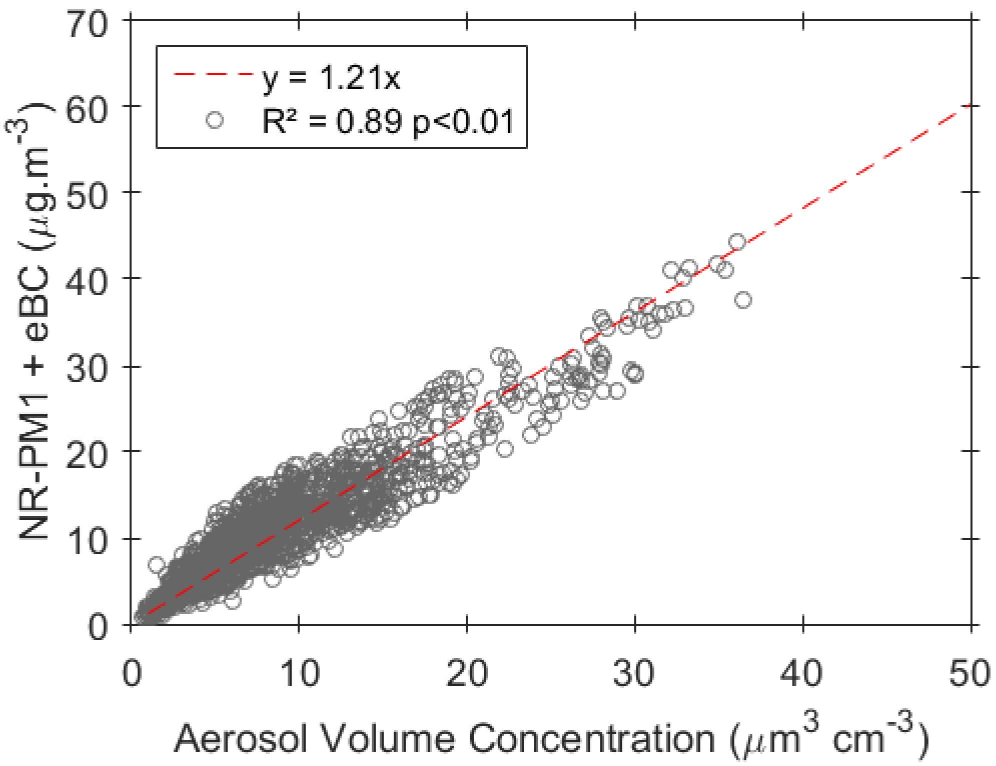

Figure S6 - Comparison of the PM_1 mass concentration (ACSM plus MAAP) with the aerosol volume concentration derived from the SMPS.