Reply to the referees and the editor

We thank the editor and all reviewers for the thorough revision of the manuscript and the feedback focusing on the readability of the manuscript. We acknowledge the technicality of the manuscript, aiming to properly describe the methods used to make them replicable by the audience. However, we recognise the manuscript could be more accessible in the method presentation, as also further stressed by the editor, and we attempt in this revision to make it more reader-friendly.

Hence, we have addressed all comments provided by the referees and will be presented here in a point-by-point manner but also made some modifications to further clarify the text. All the corrections are presented in blue font and are marked in the manuscript with the tracking changes tool.

Minor corrections

1. **Figure 1: Make the markers strictly vertical lines to improve visibility and comparability, and apply this consistently to all similar graphs.**

Figure 1 and all the rest of the pertinent figures have been modified as suggested using vertical lines to indicate the truth values instead than a marker. The figures are shown below:

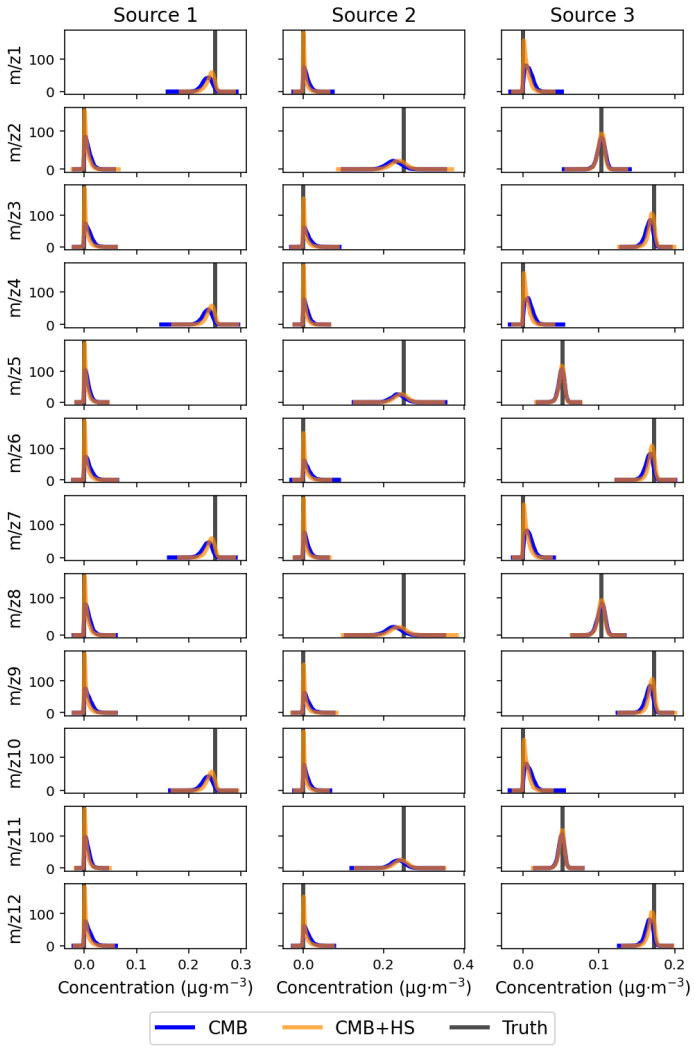


Figure 1. Distributions for the mass concentrations of all measured variables (m/z) for both CMB and CMB+HS (solid lines) compared to truth (markers).

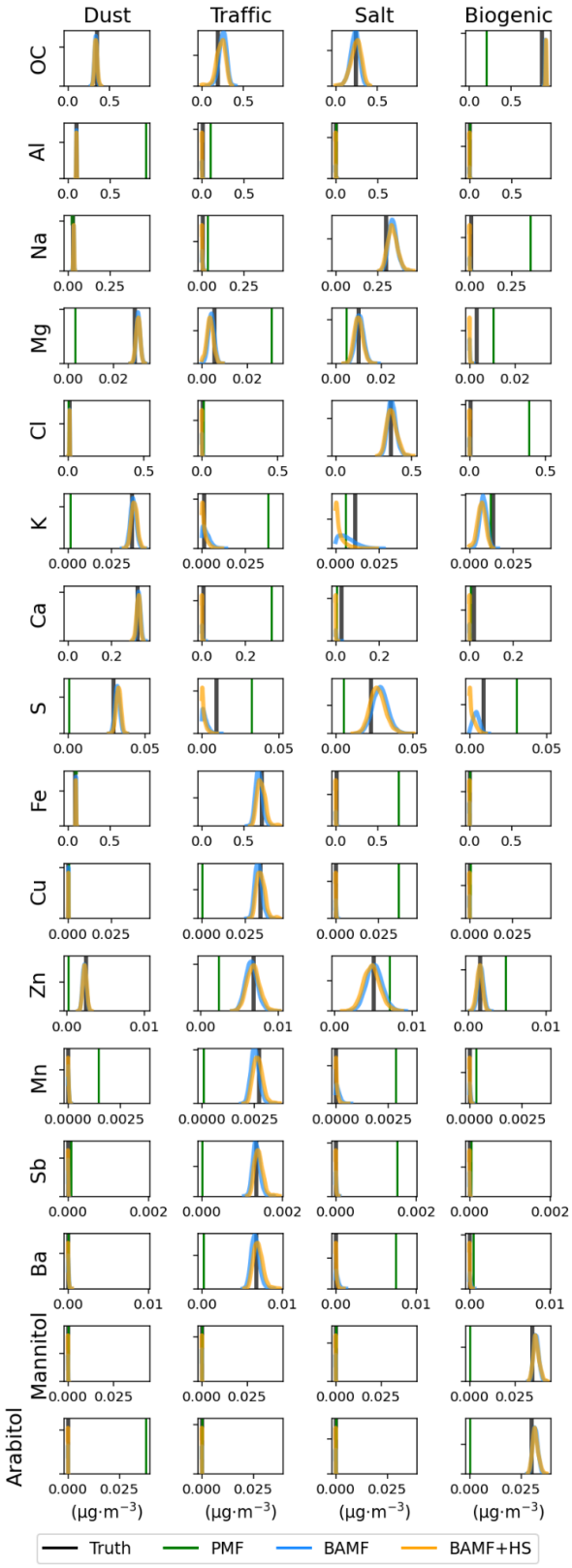


Figure 4. Profile components distribution for PMF, BAMF, BAMF+HS (colored lines) in comparison to the truth (black lines) on the real-world filters dataset. Rows represent the species of the source apportionment and columns represent sources.

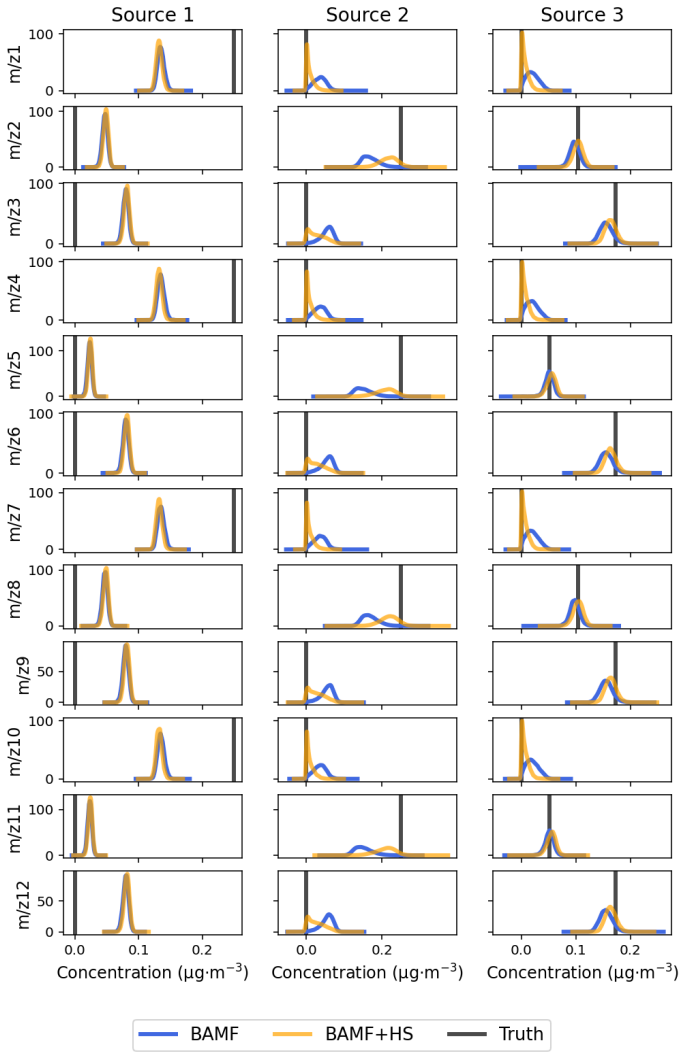


Figure S5. Toy dataset distribution of F components for BAMF, BAMF+HS.

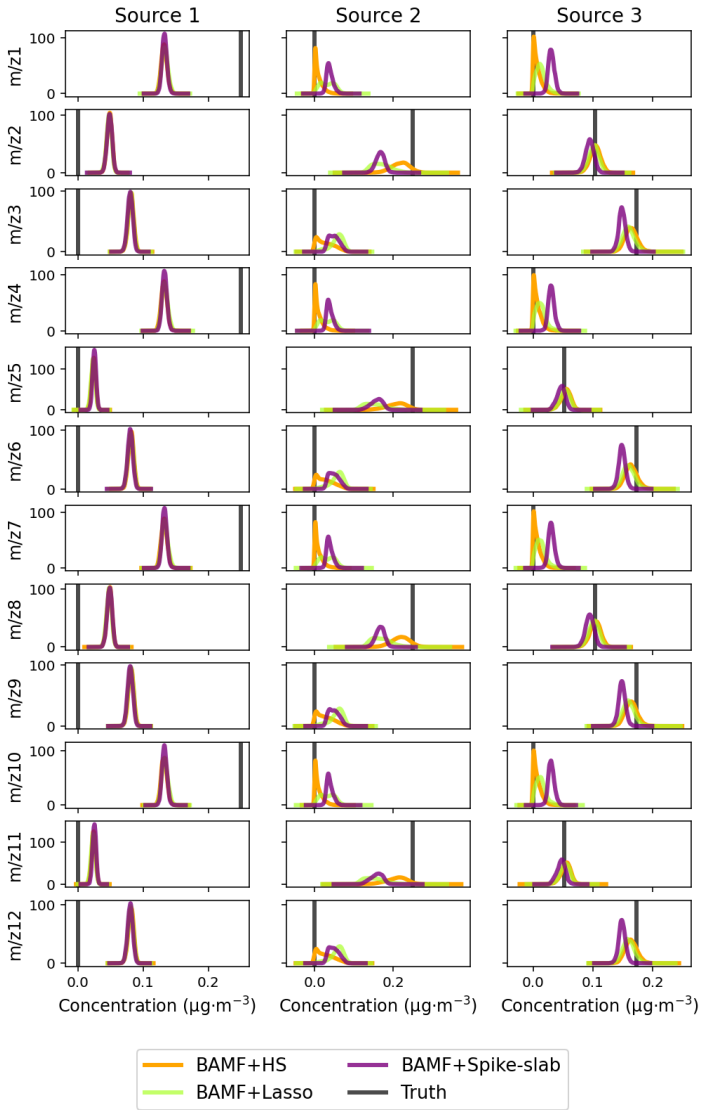
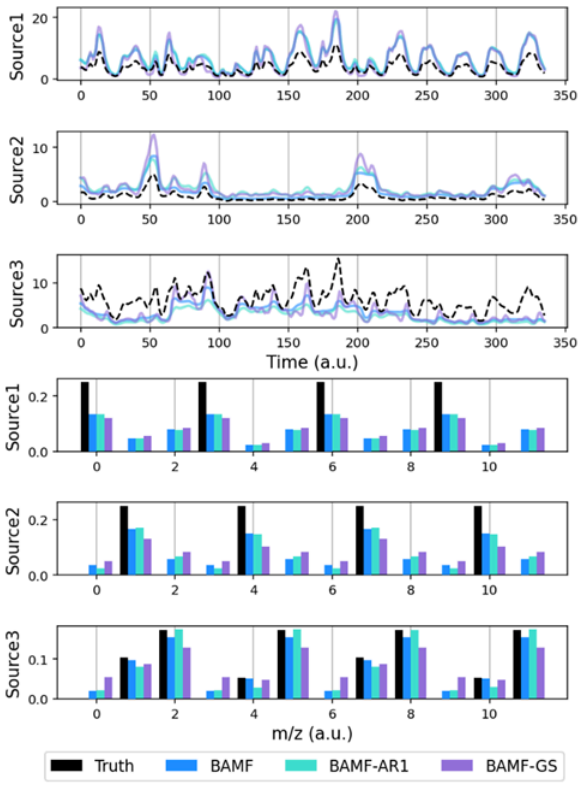


Figure S6. Comparison of toy dataset distribution of F components for BAMF+HS, BAMF+Lasso, BAMF+Spike-and-slab.


Source1
Source2
Source3
Time (a.u.)
m/z (a.u.)
Truth
BAMF
BAMF-AR1
BAMF-GS

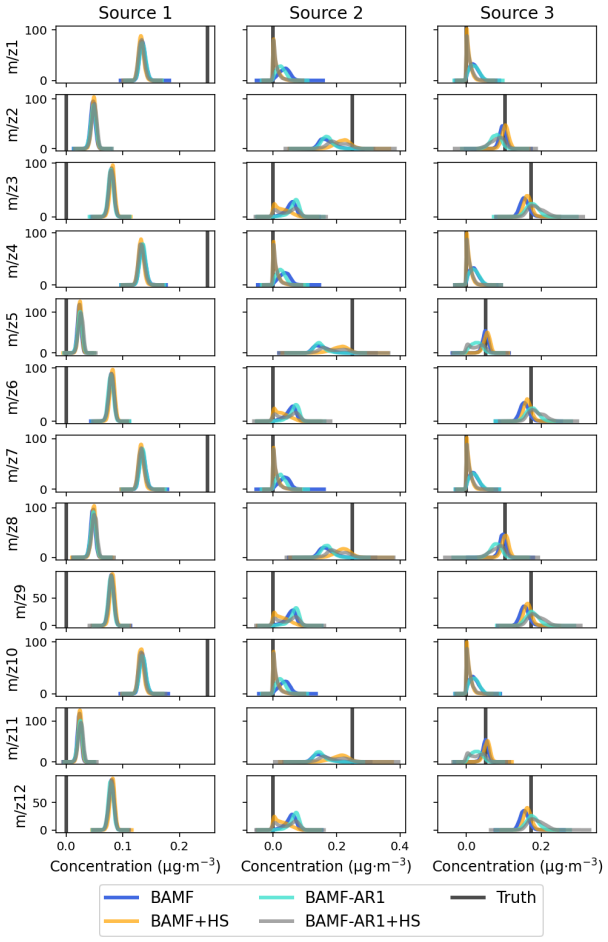

Source 1
Source 2
Source 3
m/z1
m/z2
m/z3
m/z4
m/z5
m/z6
m/z7
m/z8
m/z9
m/z10
m/z11
m/z12
Concentration (μg·m^{-3})
BAMF
BAMF+HS
BAMF-AR1
BAMF-AR1+HS
Truth

Figure S7. Left: Toy dataset time series (top) and profiles (bottom) results with BAMF, BAMF-AR1 and BAMF-GS. Right: Toy dataset distribution of F components for BAMF, BAMF+HS, BAMF-AR1, BAMF-AR1+HS.

2. **Figure 1 caption: Consider revising to: "Distributions for the mass concentrations of all measured variables (m/z) for both CMB and CMB+HS (solid lines) using the toy dataset."**

This change has been applied as follows:

Lines 854-855: **Figure 1. Distributions for the mass concentrations of all measured variables (m/z) for both CMB and CMB+HS (solid lines) compared to truth (markers).**

3. **Figure S1: Improve the resolution and spell out acronyms in the caption, such as MCMC.**

We increased the resolution of the picture and added the acronym spelling in the figure. The improved version of Figure S1 is shown below:

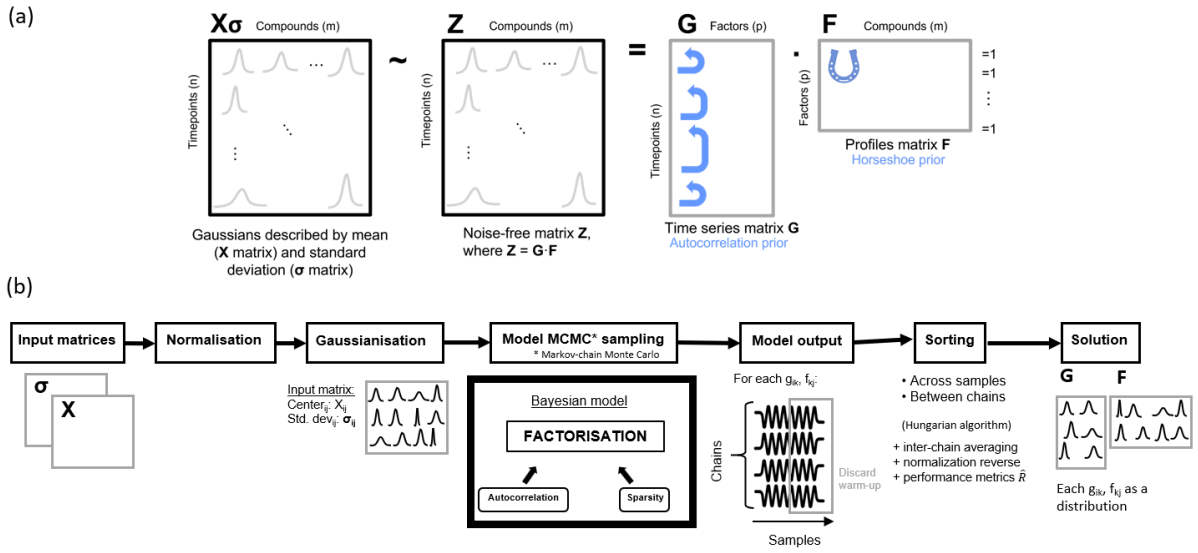


Figure S1. (a) Bayesian matrix factorisation for source apportionment sketch with autocorrelation and horseshoe priors. (b) Workflow diagram showing the aerosol source apportionment stages with the BAMF+HS model. This figure portrays the previous and posterior processes to the MCMC sampling, and both starting and end points. Concepts as chains and samples, mentioned in the text, are schematised in the workflow as well.

4. **Figure 2: Spell out "a.u.", as it may be interpreted as other units (e.g., astronomical units, the distance from the Earth to the Sun). Since you mention m/z in the toy dataset elsewhere (e.g., Fig. 1), it would be helpful to add "(arbitrary units)" after all instances.**

Figure 2 has been modified as recommended, spelling out the 'a.u.' acronym.

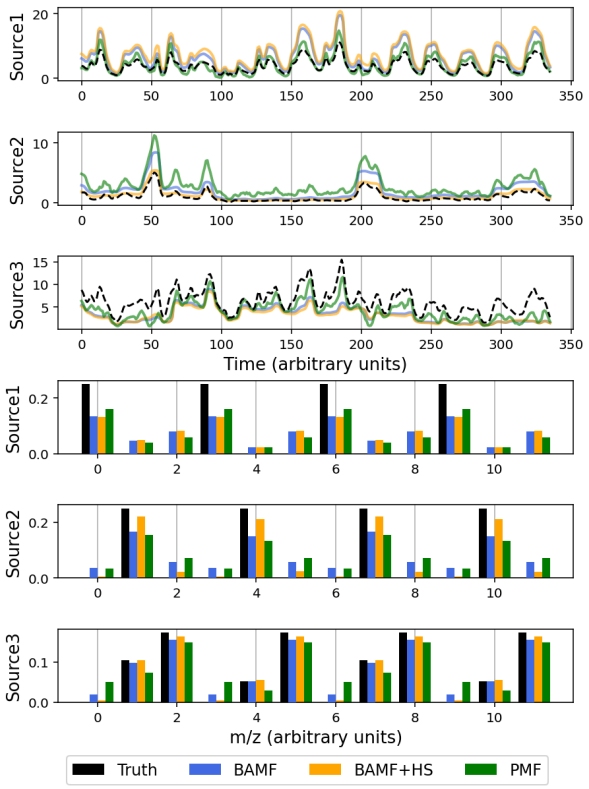
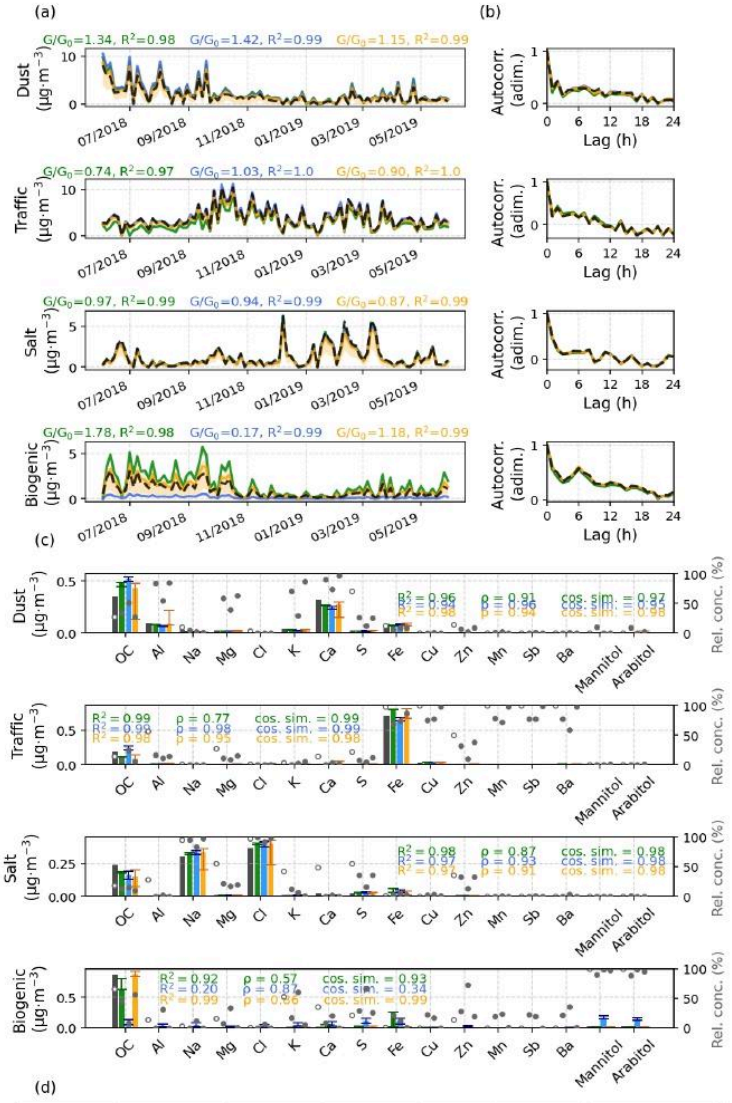


Figure 2. Source apportionment results for the toy dataset obtained using PMF, BAMF, and BAMF+HS, compared against the true solution (black bars). (a) Factor time series. (b) Factor profiles.

5. **Figure 3: The legends containing G/G_0 and R^2 are obstructing the figures. Consider placing all three model legends in a single line at the top of the graph.**

Figure 3 has been adapted to place the time series statistics on top of the time series subfigures so that the text does not obstruct the time series. Below, the corrected figure is shown.



Factor	Model	F contr. R^2	F contr. ρ	F Gini	F Gini ratio (*)	Truth zeros sum
Dust	PMF	0.95	0.84	0.79	0.90	0.0035
	BAMF	0.77	0.90	0.80	1.08	0.0025
	BAMF+HS	0.94	0.90	0.79	1.07	0.0011
Traffic	PMF	0.99	0.90	0.89	1.19	0.0000
	BAMF	0.93	0.94	0.85	0.99	0.0005
	BAMF+HS	0.995	0.93	0.88	1.02	0.0004
Salt	PMF	0.95	0.84	0.79	0.90	0.0012
	BAMF	0.95	0.88	0.80	1.01	0.0118
	BAMF+HS	0.98	0.87	0.82	1.04	0.0031
Biogenic	PMF	0.87	0.43	0.85	1.08	0.0035
	BAMF	0.53	0.51	0.50	0.56	0.0118
	BAMF+HS	0.96	0.84	0.90	1.01	0.0007
$\sum_k$ (*)	PMF	3.80	3.04	3.34	0.43	0.0198
	BAMF	3.18	3.23	2.95	0.53	0.0172
	BAMF+HS	**3.88**	**3.54**	**3.39**	**0.15**	**0.0031**

Figure 3. Synthetic offline dataset source apportionment results for PMF, BAMF, and BAMF+HS models. (a) Time Series. (b) Autocorrelation. (c) Profiles. (d) Table with additional metrics for comparison to truth.

Bold numbers reflect the highest value amongst models. F contr. represents here the percentage of each factor in a given species. The sum row reflects the overall performance of the model for all sources for each statistic metric except for the ones marked with (*), in which the difference to 1 in absolute value is summed up.

6. **Figure 5: Include a percentage sign on the y axis for the profiles.**

The percentage sign was added on the right axis of Figure 5 for the sake of plot readability.

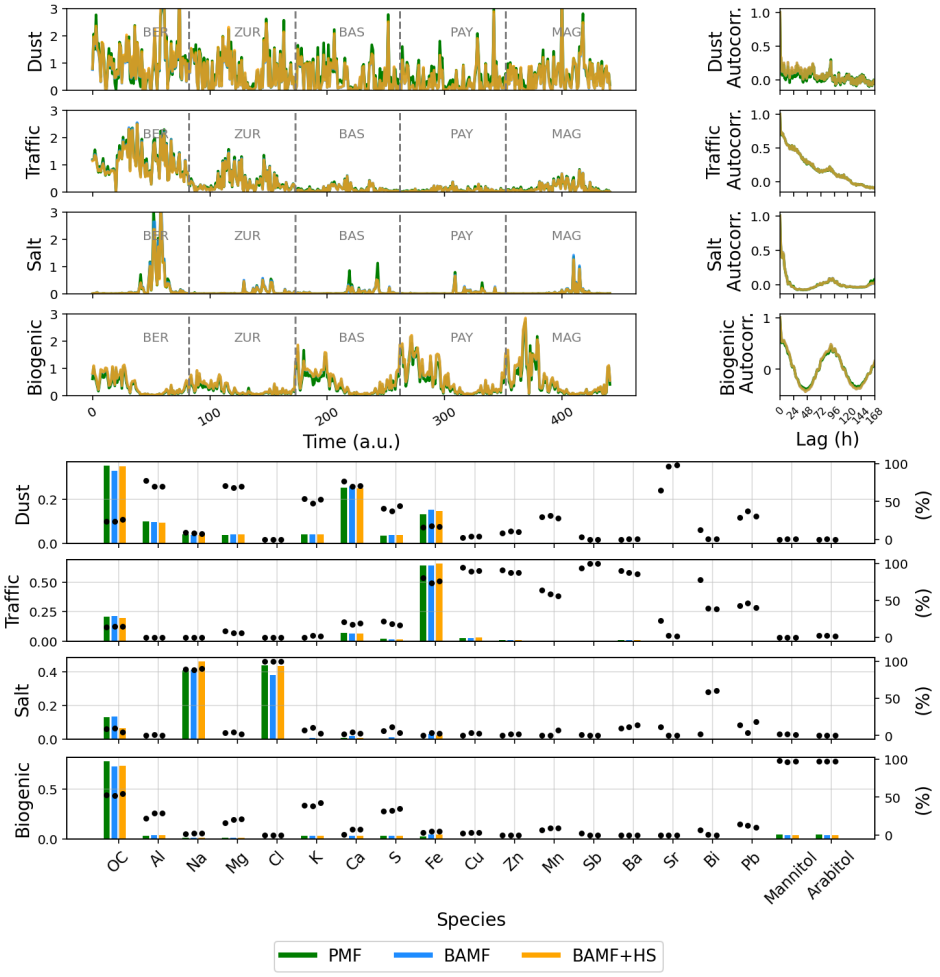


Figure 5. Comparison of PMF, BAMF, BAMF+HS for the real-world filters dataset. From left to right and top to bottom: time series, autocorrelation, and profile plots. The dots in the profiles (right axis) show the contribution of each species to the source.

Further clarifications

1. **We added some clarifications in the BAMF model section for the sake of clarity to the reader:**

Lines 119-121: "... With that formulation, the measurements matrix **X** is modeled into a Gaussian

distribution whose centre is the **G** · **F** product matrix and its standard deviation is the uncertainty matrix **σ**. In turn, one introduces certain restrictions on the **F**, **G** matrices characteristics in the form of priors. ...”

Lines 136-139: “... The imposition of autocorrelation in **G** entails that two consecutive measurements should be more similar than two measurements apart in time, and that the similarity should fade with the temporal gap between them. This property is particularly advantageous for atmospheric pollution dynamics, which, generally, are expected to exhibit temporal smoothness rather than abrupt fluctuations. …”

Lines 153-154: “... Here we propose a sparsity enforcement into the profiles matrix, intending to remove small contributions of irrelevant species for a given factor. …”

2. **We further guide the audience on what is the purpose of the developed models in:**

Lines 226-228: “... The objective of the inference is to retrieve the parameters of the model, primarily **F** and **G** but also all the other defined parameters (τ, λ, α, β**).** These are sampled from their posterior distributions, constructed from the priors and the data introduced. ...”

Lines 232-234:”... Accepted positions correspond to plausible parameter values (of the **F**, G, τ, λ, α, and β parameters in our case) given both the model assumptions and the data. “

3. **More clarifications.**

Lines 71-73: “ In this approach, the mass closure condition was taken to the Bayesian framework and an autocorrelation prior, AR(1) (the first order autoregression formulation), was applied, improving the solution given assuming independent **G** components. “

Lines 274-275: “... In the model outcomes, the factor ordering in the matrices is random in the model results, hence, the solution factors must be sorted. …”

Lines 178-181: “... The distribution parameters τ_0, σ_{HS}, and slab_df, slab_scale were tested and results did not show significant sensitivity to their variations, so we keep the default ones as provided in Piironen and Vehtari (2018) in their available shared codes. …”

Lines 187-190: “... It is a proxy for how deviant a dataset is from the total equality amongst its components. Since it quantifies the inequality, it can be a proxy for sparsity; if some values are high and the others are zero, Gini ≈ 1 (great inequality), if all values are equal, Gini = 0. ...”

Lines 660-661: “... The regularised horseshoe prior, a tool to promote sparsity in datasets, is introduced in BAMF (BAMF+HS) in order to narrow down the lowest signals in factor profiles while keeping the most significant ones regularised. …”