Author's reply to peer-review comments on
"Associativity Analysis of SO2 and NO2 for Alberta Monitoring Data Using KZ Filtering and Hierarchical Clustering" by Joana Soares et al. submitted to ACP

Dear Anonymous **Referee #3**,

We are grateful for your efforts and the overall positive evaluation of our manuscript. The constructive comments have helped us to further improve our paper. Below we give our detailed responses to your comments and describe the revisions prepared for the manuscript. The Referee comments are cited in italics and our responses in regular type while revisions prepared to the manuscript are marked in red.

General and specific comments:

1) The abstract is too long and can be shortened only giving the key results and a recommendation to follow.

- The Authors have shorted the abstract: "Associativity analysis is a powerful tool to deal with large-scale datasets by clustering the data on the basis of (dis)similarity, and can be used to assess the efficacy and design of air-quality monitoring networks. We describe here our use of Kolmogorov-Zurbenko filtering and hierarchical clustering of NO_2 and SO_2 passive and continuous monitoring data, to analyse and optimize air quality networks for these species in the province of Alberta, Canada. The methodology applied in this study assesses dissimilarity between monitoring station time series based on two metrics: 1-R, R being the Pearson correlation coefficient, and the Euclidean distance; we find that both should be used in evaluating monitoring site similarity. We have combined the analytic power of hierarchical clustering with the spatial information provided by deterministic air quality model results, using the gridded time series of model output as potential station locations, as a proxy for assessing monitoring network design and for network optimization. ~~We find that both metrics should be used to evaluate the similarity between monitoring time series, since this allows a cross-comparison in terms of temporal variation and magnitude of concentrations to assess station potential redundancy.Here, the relative level of potential redundancy of an existing monitoring location was ranked according to each dissimilarity metric, with sites forming clusters at low values of both 1-R and Euclidean distance being the most redundant.~~ We demonstrate clustering results depend on the air contaminant analyzed, reflecting the difference in the respective emission sources of SO_2 and NO_2 in the region under study. Our work shows that much of the signal identifying the sources of NO_2 and SO_2 emissions resides in shorter time scales (hourly to daily) due to short-term variation of concentrations, and that longer term averages in data collection may lose the information needed to identify local sources. However, the methodology ~~nevertheless~~ identifies stations mainly influenced by seasonality, if larger time scales (weekly to monthly) are considered. ~~We have found that data consisting of longer-term averages may lose the short-term variation needed to identify local sources, implying that long-term averaged observations are not suitable for source identification purposes. In addition to averaging time, round-off levels in data reports, and the accuracy of instrumentation were also shown to have a negative influence on the clustering results.~~ We have performed the first dissimilarity analysis based on gridded air-quality model output, and have shown that the methodology is capable of generating maps of sub-regions within which a single station will represent the entire sub-region, to a given level of dissimilarity. ~~Maps of this nature may be combined with other georeferenced data (e.g. road networks, power availability) to assist in monitoring network design.~~ We have also shown that our ~~methodology~~ approach is capable of identifying different sampling methodologies, as well as identifying outliers (stations' time series which are markedly different from all others in a given dataset)."

2) Can the authors explain why they consider only SO2 and NO2?

- This manuscript focused only on NO_2 and SO_2 because only these two species had both passive and continuous monitoring data available, as mentioned in P3, L34-35 "We analyse data from both passive and continuous instruments measuring NO_2 and SO_2 ambient concentrations, the two species that include observations from both measurement methodologies." We have examined other continuous data using the methodology, and intend to discuss these other air contaminants in future work. We revised the text to make this clearer in the manuscript, viz:

  P3,L34-35 "In this study we included observations ~~We analyse data~~ from both passive and continuous instruments measuring NO_2 and SO_2 ambient concentrations, since these are the only two species in the available data that include observations from both of these measurement methodologies."

3) *In the introduction, between lines 25-39, the authors only list the available literature but do not make a synthesis of these results and link it to their motivation of doing this study. What was missing in these studies?*

- The authors wanted to describe the scientific work using cluster analysis of observational data that apply the same metrics used in this study. We are not implying that is missing something in the referenced work, we wanted to illustrate how cluster analysis techniques have been used for different species and locations. The text was revised to accommodate this comment.

  P2, L33: "oxidant (O_x), non-methane hydrocarbons (NMHC), and PM. In this past work, cluster analysis is usually applied to a small number of stations (5 to 70) in different locations around the globe. Solazzo and Galmarini (2015) applied cluster analysis data pre-filtered by iterative moving averages (Kolmogorov-Zurbenko (KZ) filtering, Zurbenko, 1986). Their work showed that cluster analysis can potentially accommodate different sampling technologies, and could be applied for large areas without the need of prior knowledge of the study area. Here, Solazzo and Galmarini (2015) applied cluster analysis data pre-filtered "

  P3, L4: "(2015) and references therein, and further expands that methodology to focus on monitoring network optimization. We use the methdology for the first time for observation datasets collected in Alberta, analysing the data using two different similarity metrics, and rank existing observation stations based on relative station redundancy. We then extend the methodology to a new application of gridded air-quality model data – showing that time series from a deterministic air quality model (Global Environmental Multiscale – Modelling Air-quality and Chemistry; GEM-MACH) may be used as a surrogate for observations in air-quality clustering analysis. ~~The methodology uses the time series of observations at different monitoring stations in Alberta, and analyses this data based on two dissimilarity metrics~~. Dissimilarity may thus be used to rank stations in terms of potential redundancy, where stations having the lowest levels of dissimilarity may be considered sufficiently similar to be considered potentially redundant.

~~In addition, we apply the same methodology to time series from a deterministic air-quality forecast model (Global Environmental Multiscale – Modelling Air-quality and Chemistry; GEM-MACH) and assess the extent to which the model output can be used as a potential surrogate for observations in clustering analysis~~ The combined use of deterministic model output and clustering analysis is shown to be a potentially powerful tool for network design, and/or optimization of existent air quality networks.

4) Is it not possible to higher in resolution in the modelling part as 2.5 km resolution might be coarse for the purpose of the study? I think this deserves a discussion.

- The potential use of even higher resolution (1km) was examined in separate work. The results were inconclusive in that higher resolution does not guarantee a more accurate air-quality forecast. For example, if the predicted synoptic or mesoscale meteorology is inaccurate due to poor spatial representation of a region in the meteorological monitoring network, then the benefits of higher resolution in air-quality simulations (resolving the sources to a higher degree) may be overwhelmed by the issues associated with highly resolved plume locations being inaccurately predicted. There are also practical computational considerations – to carry out the same domain simulations as carried out here would have required a 6.25x increase in processing time and memory.

5) Figure title of S6, S7 and S8 are wrong, please correct them to SO2.

- The authors noted that the dendograms are actually for NO_2 and not for SO_2, as it should be. The figures were revised.