Interactive comment on “Application of Factor and Cluster Analyses to Determine Source–Receptor Relationships of Industrial Volatile Organic Odor Species in a Dual-Optical Sensing System” by Jen-Chih Yang et al.

Anonymous Referee #1

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The study “Application of Factor and Cluster Analyses to Determine Source–Receptor Relationships of Industrial Volatile Organic Odor Species in a Dual-Optical Sensing System” by Jen-Chih Yang et al. uses FTIR spectroscopic measurements to determine the source of the emission of Volatile Organic Odor Species near an industrial park in southern Taiwan. The measurements are carried out at three sites (CY: a sun glass factory, KS: a light metal casing factory, NS: solar cell manufacturer), where the odor and contamination might be emitted and another where the odor and the related species are detected. Therefore in this study the composition of the stack emissions...
from three different industrial complexes are characterized using closed cycle FTIR-spectroscopic measurements and at another time the pollution event with its characteristic odor species using open path FTIR spectroscopy using a retroreflector and 2x143m pathlength. FTIR spectroscopy allows the determination of the concentration from various gases and is very suitable for this purpose.

Here the technique in both geometries (closed cell measurements and open path) might allow according to the authors the determination of more than 300 pollutant species using the commercial software based on linear least square fitting. At least 17 species are indeed detected and reported in table A1 and figure A3 of this study. The contribution of the different sources to the pollution events are identified by their specific composition, emission profile or here named Factors F_i. Therefore different industrial processes are related with a specific combination of different pollutants. This combination are obtained using the two statistical method: Factor analysis and Cluster analysis.

The technique which allows for the simultaneous measurement of different gases is very suitable for the “Factor analysis” and the determination of different emissions profiles produced by different processes and the Cluster analysis as well the meteorological data confirm these findings.

The approach which allows to identify the different sources and determine sus contributions to the odor quantitatively is interesting, meets the scope of the journal, is in general well written and therefore suitable for publication in AMT after some revision in more detailed described below and after providing some more detailed information.

General: The strength of the article is the nice an clear concept using FTIR measurements which allows for the measurement of 17 species simultaneously, measure “emission profiles“ of these species at the potential sources using cell measurements and detect these emission profiles at the receptor site using open path measurements and compensate the dilution using an increased path length. The statistical methods
are chosen in a proper way and the results are clear. In addition the study also is able to determine different industrial processes, which are occurring at the three odor producing sites, and the meteorological conditions, which confirm the identification of the origin of the odor of different events. The structure of the article might be logical, but the references to the figures in the text is sparse and might be missing sometimes and the use of T1 and TA1 as well as Figure 1 y Figure A1, without adding an Appendix with a text document is confusing and make it a bit difficult to understand the article. Therefore work is required to improve the manuscript and its readability before publication.

There are some questions, which are not easily to answer, but it should be clear for the reader: 1.) Two set up are used but to my understanding it would work also with just one FTIR, as the measurements at the potential sources are realized independently and also the open path measurements at the two sites do not have to be simultaneously. 2.) Factor and cluster analysis are two independent methods: Are they used to confirm each other, compliment some aspects or as “combined” analysis 3.) Which role-plays the meteorology in the analysis? The meteorological data might also be used in the cluster analysis or are only used to confirm the other method in the different cases. Especially here you use the different factors to confirm that the method works proper and you can get the sources from the factors.

0. Abstract: Maybe the author could already state in the abstract the location and time where the measurement where taken. This study developed and alternative approach and an dual. . . Air contaminants in and nearby a industrial park in southern Taiwan. 

line 6 page 2 “Continuous monitoring” alone is a bit misleading, if you talk about both receptor site and source emissions, because it implicitly say “simultaneously”, which is not the case. Maybe you can add just the periods where sources and where receptor sites are “measured continuously”. Or just add “during different periods”

2. Materials and Methodology:
1.1 Site description and sampling techniques Page 4, line 14-page 5 line 19

I would recommend to separate “Site description” line 16-26 and “sampling techniques” line 27-19

Please could you add a map with all sites and distances.

Measurement method:

The end of the introduction already gives description of the method, for me that is ok, but please add there or here the very important information about the path length in the “Closed Cell” the used pressure in the cell and a estimation of the gas flow through the cell. Did you try to reduce the water vapour to decrease interference with H2O absorption or is it not necessary.

2.2 Chemical analysis methods

There is no always a link to the figures and tables, but from the table 1 it can be seen that you found 17 relevant species, this is more interesting than the list of species in the library. I would recommend move the parts of the description of the technique from the Instrument manual to the introduction (e.g. more than 300 species) and the concrete chosen settings and the indeed used species in the method- section. It would be nice to get the complete set of 17 micro windows, where the 17 species are retrieved also in a Table as Figure 3A has very small characters at the x axes and shows only 16 species.

How the rolling background is calculated and used should be explained more detailed.

2.3 Qualitative receptor modelling: It is not very clear described. What is the index in $X_\cdot$, $X_1$, $X_2$ in Eq 1-4. Or the first index in the coefficient $a_{11}$. I would assume the index $X_1 = X_t1$ and describe the time of the observations, as the origin of the Factors $F1,\ldots$ is not stated it seems to be taken from the OP-observations. I would like something like $F1_{op}$ (open path 1) and maybe an corresponding Factor $F1_{CY}$ or $F1_{NS}$, $F1_{KS}$. So it is very clear. And please report the factors at the receptor site C4.
and the source sites in a comparable way. Maybe complete the factors in table 3 as they are in table 2 just by adding 0.0. And please add the Factors from the site NS to table 3.

Maybe you could also report a table with the scalar-products of \( <F_1_{\text{CY}}, F_2_{\text{OP}} > \) for the 4 open path factors \( F_{i\text{OP}} \) with all source factors. Just taking Table 2 and table 3 (after adding the NS factors) would be a \( 4 \times (2 + 2 + \text{factors NS}) \) Table/Matrix. It would even be interesting, if the factors of the different sources NS, CY, KS are more or less orthogonal or have a strong overlap.

3.2 Ambient data from receptor path:

Please add a Figure with the time-series which are the basis for the calculation of \( r_{\phi \text{phi}} \) and \( r_{p b} \), OP-FTIR measurements and indicate, when odor was reported. Figure 2 shows no values, when the factor might be negative, please correct it, even if the contribution of the factor is negative it has to be reported. There should be errors in the coefficients, which explain negative values at least in a small range. Caption Figure 2: Time-series pattern –> Diurnal time-series pattern

Missing Figure: Could you add a complete time series of the 4 factors found at the receptor site, which is not a diurnal pattern

4. Conclusions: Is a bit short and very arbitrary and a little redundant.

p. 10 l. 17: I would replace “dual-optical sensing system” by “FTIR- spectroscopic measurements.” And clarify less ambivalent how the meteorological data and cluster analysis was used. Maybe something similar as: “This study developed an alternative investigative framework for detecting air pollution sources of odor nuisance by measuring 17 gas species simultaneously using FTIR spectroscopic measurements and factor analyses to identify and characterize emission sources of multiple air contaminants. Meteorological data and Cluster analyses were employed to proof the identification of the major odor emissions” Maybe you could add some numbers how often the odor
occures which originate from CY, KS, NS and the different processes.

Figures and Table: Please do not use Appendix if you refer to the figure or table in the main text and ensure that all figures and tables are mentioned in the text and keep the order how they are used in the text.