

Interactive comment on “Identification and Source Attribution of Organic Compounds in Ultrafine Particles near Frankfurt International Airport” by Florian Ungeheuer et al.

Anonymous Referee #2

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General comments. This manuscript presents an analysis of the chemical composition of the ultrafine particle fraction of aerosol samples collected downwind of a major airport. The authors used a non-targeted screening approach to identify ~ 200 chemicals that were more than 5 times the signal observed in the blank. The majority of the compounds were attributed to jet engine lubricating oils based on molecular formula, MS/MS fragmentation, retention times in a UHPLC column, and a comparison to standards from jet engine oils. The data analysis is thorough and the paper is well written. However, there are places where additional information should be included and clarifications given. I recommend this for publication in ACP after the following specific comments are addressed.

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Specific Comments 1. In the experimental it is stated that “Pure organic solvents provided the higher extraction efficiency than mixtures with water and similar ones to mixtures of acetonitrile and methanol.” How was the extraction efficiency quantified and was it compared across different types of molecules, or only across the ones that are extracted well with the solvent that was chosen? What were the different pure organic solvents that were tested?

2. In the experimental it is stated that “A circular section with a diameter. . .according to the array of the nozzles of each impactor stage”. Can you please clarify what this means? Were specific areas of the foil targeted?

3. In the discussion of the UHPLC/HRMS method it is noted that the two standards that were tested had a small linear response range “likely due to their adsorptive behavior on glass surfaces”. If these are representative of the types of molecules found in this work, how likely is it that the other chemicals may have been influenced by this as well? I recognize that quantification was not attempted for the other compounds, but I would suggest adding a note to this effect given that qualitative comparisons of peak areas were carried out.

4. In the results and discussion it is noted that “the majority of these compounds does not distinguish from the blank”. Does this mean that the majority of the compounds were also measured in the field blank? Were laboratory blanks also run and were these clean of the chemicals? Is this contamination occurring in the field, or is this coming during the sample handling/processing?

5. It is noted that the program provides a false assignment for the pentaerythritol esters. On page 10 it is written that: “The native molecular fingerprint is displayed in Figure S4”. What does this mean? Are these the results using the false assignments? If so, why is this being shown? If not, please clarify what this means and what is being plotted in Figure S4.

6. It is noted that the O/C ratios are below 0.6 and thus that the UFP do not become

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oxidized during transport. Please provide the O/C range for the starting material to support this (from Figures S6-S10).

7. On page 15: "Although no tri-ortho isomer of TCP was detected, it is still to consider that isomers with only one ortho-methyl group feature possibly a higher toxicity than the meta- and para-isomers. . .". I am unsure what is being communicated here and suggest rephrasing.

Minor comments:

8. Please add a note that this is positive ion mode in the caption for Figure 2 (unless it includes both positive and negative ion mode, in which case please clarify that).

9. There is a darker purple in Figure 3 A and D that is not present in Figure 3 B and C. I think this is just a shading issue, but I recommend correcting it so that all the colors match the key.

Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2020-1091>, 2020.