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Comment

# ***Interactive comment on “Characterisation and optimisation of a method for the detection and quantification of atmospherically relevant carbonyl compounds in aqueous medium” by M. Rodigast et al.***

**Anonymous Referee #1**

Received and published: 19 February 2015

In this study the authors present an optimized analytical method dealing with the quantification of carbonyl compounds. The carbonyl compounds chosen for the method optimization include atmospherically relevant species from primary and secondary sources. Optimized method parameters include concentration of derivatization reagent, derivatization time, pH during derivatization and extraction, extraction time, and extracting reagent. Thus, a comprehensive optimization of the sample preparation was carried out followed by a standard GC/MS analysis. Due to this comprehensive evaluation of parameters and the choice of relevant carbonyl compounds I think the

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paper is well suited for publication in AMT. However, organization and presentation of the paper should be improved prior to publication as outlined in the specific comments below.

Specific comments:

1. Apparently, the optimizations presented in this study are limited to the sample preparation part of the analytical procedure to detect and quantify atmospheric carbonyls. This should be better reflected in the title of the manuscript.
2. A clear (short) description of the overall analytical procedure is missing in the experimental section of the main text. The GC/MS analysis is only mentioned in the abstract and in the captions of Figure 2 and Table 3.
3. The first two paragraphs of the results section on page 861 need to be revisited for language and clarity. The first sentence of the first paragraph is good examples for this point. In my opinion this sentence should read something like “Studies reporting optimized methods for the quantification of carbonyl compounds including a PFBHA derivatization procedure are summarized in Table 1”. The first two sentences of the second paragraph could be removed without a loss of information, if the parameters optimized in this study would be included in the next sentence.
4. In my opinion the paper will be better perceived by the community if analytical parameters like the relative standard deviation (RSD) of repeated injections (repeatability of the measurement) would be given, e.g., in Table 3. Also, error bars are missing in Figure 2b. In Figure S7 (calibration curves) it is not clear to me what is meant by the x-axis label “theoretical concentration”. Were the injection volumes or the actual standard concentrations varied? In general, Table and Figure captions as well as subsection headings should be revised for clarity and readability.
5. The discussion on the influence of extraction time (3.2) is very interesting, as variations from the extraction times reported in other studies might lead to a decreased

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reproducibility of the results, if the extraction is not >99% complete after 2-3 minutes.

6. Personally, I would rename subsection 3.6 into “Proof of principle”. The first paragraph of this subsection could go to the experimental section and/or to supplement section 2.7.

7. Section S2.1 and Table S1: I would limit the overview of applications of PFBHA derivatization techniques used in carbonyl analysis to those relevant in the atmospheric context, but extend it to be more comprehensive. In my opinion this would be of greater interest than listing applications of methods optimized for the analysis of carbonyls in other fields.

Exemplary technical comments:

P. 858, L. 7: This sentence should be removed

P. 858, L. 8: Please clarify or remove this sentence, too

P. 858, L. 14-16: Should be changed to “Detection limits between 0.01 and 0.17  $\mu\text{mol}$  L<sup>-1</sup> were achieved, depending on the carbonyl compound”

P. 858, L. 16-18: This sentence reads like extraction was carried out before derivatization.

P. 858, L. 21-22: The yields reported here are not final yields but yields after 5h of reaction. This should be clarified.

P. 859, L. 23: “better quantification” should be specified

P. 860, L. 18-20: This sentence needs to be clarified. What is meant by standard compound for method development – I assume the corresponding experiment was used as a proof of principle

P. 861, L. 1-2: This sentence should be improved for a better readability. How much PFBHA (mL or g) was added to the sample to achieve the final concentration of 0.43

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mg mL<sup>-1</sup>.

Supplementary Information:

P. 1, L. 18: Heading could be “GC/MS analysis”

P. 1, L. 28: Heading could be “(Exemplary) Analysis of carbonyl compounds (in an atmospheric context?) involving PFBHA derivatization methods” (see comment #7)

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Interactive comment on Atmos. Meas. Tech. Discuss., 8, 857, 2015.

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