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Atmospheric Measurement Techniques
Discussions

Interactive comment on "The influence of the baseline drift on the resulting extinction values of a CAPS PMex" *by* Sascha Pfeifer et al.

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We would like to thank the Referee for the constructive comments.

Response to the general comments:
The referee has two relevant critical points. First, a more detailed description of other alternatives, especially hardware based solutions. Furthermore, any limitations of the correction method are not sufficiently described. Both points are generally legitimate remarks.

It is undisputed that a functioning hardware based solution is preferable to a software-

based correction. However, it should be emphasized that this correction method is a simple method without any additional cost and effort to optimize the measured values. In addition, it is even possible to optimize old existing data sets in a post-processing. For the reasons given above, we consider this method to be useful.

The aim of this article is not to gain "ingenious novel insights". The focus of this article is to describe the effect of the baseline drift on the resulting extinction values, exemplary for an urban background station. The intention is to analyze the artefacts and to present a simple method to reduce these effects. This is in the sense of a technical note.

We have tried to consider the points of criticism, without expanding or shifting the focus of the article.

Please find our response to each of the specific comments below:

The suggested correction scheme works for the example data provided. However it will not work as effectively when there is significant variability in NO2 between consecutive baseline measurements. Indeed, it would appear possible that in some circumstances the applied correction could make the bias worse compared to the standard method (e.g. where the baseline increases between consecutive baseline periods but gaseous absorption decrease in the interim period). For this reason I question what applying this new correction really enables users to say with confidence about the accuracy of their resulting extinction numbers. This needs to be examined in more detail in the paper.

In general, this fact is correct.

The authors are aware that any form of interpolation never leads to a gain in information. This is a fundamental fact and should be clear to everyone who uses interpolation no matter where it is used.

However, if the variability between two baseline periods fluctuates strongly, the internal calculation also fails. The internal calculation is also based on the assumption of a constant baseline for the following measuring period. In the broadest sense this is also just an interpolation, more precisely it is a forward extrapolation.

It is also correct that under extreme conditions: strongly fluctuating predictor variable with unfavourable choice of the smoothing parameter the interpolation procedure can lead to ringing/overshot structure.

However, it is important that in any case the period for the baselines must resolve the variability (this fact should be clear to the user and is even mentioned in the manual). The new procedure only allows to consider the drift or trend between two baselines. If, however, this is guaranteed, the interpolation delivers better results than the internal calculation.

To make this fact clear to the reader, the manuscript has been changed as follows:

"It should be emphasized that the use of splines interpolation to recalculate the baseline has its limits. Only trends that can be estimated from the baseline data can be reproduced for $lastbaseline$. It is impossible to reproduce any faster fluctuations that are not covered by the selected baseline period and duration. Furthermore, there is the possibility that under extreme conditions with strongly fluctuating baseline trends the method can lead to overshot structures. In these cases, the first step should be the readjustment the baseline settings."

To overcome the above, the authors suggest that users will need to tune their smoothing parameters based on the data they have, but this approach sounds unsatisfactory to me. It has worked for this study because characterising the impact of gaseous

absorbers was the focus and thus collecting long datasets while filtering was possible. In reality, people who have purchased the CAPS PMex want to be measuring aerosol extinction and thus it is undesirable to run on filter for extended periods as suggested. Indeed even if users did run with a 50% duty cycle, it still may not completely allow bias correction for reasons discussed above.

There is probably a misunderstanding here.

The filtering upstream was only done in the context of this experiment. First, to completely exclude the influence of aerosol particles on any effect. Second, to generate a reference for testing. The device should give (more or less symmetrically distributed noisy) values around zero, and no artefacts. No particle filter is required for normal operation. Just the existing data of zero period are used as predictor variables for the cubic smoothing spline. This means no additional losses of data points.

According to the comment of second referee the Fig. 2 was revised. One can see very well how the spline even reproduce the trend during a baseline measurement. We ve added this point also in text.

The corresponding section has been revised (also according to Referee 1):

"A free smoothing parameter ($spar$) must be chosen, which depends on many factors, e.g. baseline period and duration but also on sampling rate and device noise etc.. Therefore, a suitable parameter must be found for each individual device and application. For the case with 1 sampling rate, a baseline period of 5 and a duration of 1, the smoothing parameter used were 1.1, 1.3, and 1.4 for the blue, green and red, respectively. These values were determined by minimizing the artefacts of a separate test dataset. Alternatively it is also possible to determine a smoothing parameter automatically from the time series of baseline using for example the implemented generalized cross-validation method (GCV). The resulting values of the automatically calculated smoothing parameters using the GCV method do not differ significantly from the first method with values of 1.06 (blue), 1.25 (green) and 1.3 (red). Furthermore, all distinct data points with 1 sampling rate were used (all.knots=TRUE). All other parameters were set to default. A complete description of the function can be found in the R Documentation (R Core Team, 2013)."

It appears to me that there could have been scope for developing a more complex baseline correction scheme to try and overcome some of the above limitations. For example, it is shown that the red wavelength PMex units and not impacted by gaseous absorbers. Could correlations between red and green/blue wavelength units have been used to add extra constraint?

The deeper sense of such correlation is not clear to us. But as already mentioned in a point above, we refer to an alternative method to determine a suitable smoothing parameter using generalized cross-validation method (GCV).

More discussion is needed related to the realistic accuracy that applying the new corrections provides. Given the findings in the paper, how can a user quantify the accuracy of their CAPS PMex blue/green aerosol extinction measurements if they don't have a simultaneous measurement from a monitor that was run on filter?

The user can estimate the deviations by comparing the recalculated with the internal baseline values. Because the baseline correction is additive, the difference between both baseline values is the absolute deviation of the resulting extinction value. This is already explained in the text.

More discussion is needed on alternative approaches to enable reduction/elimination

of biases, including those adopted by other users (e.g. scrubbing, gas reference channels). Rather than presenting a single solution, the paper would be enhanced by presenting a range of solutions that users could consider implementing to improve the quality of their data (with accompanied discussion on the merits/complications of each).

To the best of our knowledge we don't know any no scientific publication dealing with scrubbing of NOx in a CAPS PMex.
It would probably also be accompanied by a modification of the aerosol, in particular an increase of particle losses.

A combination of gas monitor, in particular a device of identical construction, a CAPS - NO2 Monitor, in combination with CAPS PMex seems to be an alternative. DeFaria et al. (2017) combined two instruments but with different wavelength, a CAPS PMex with 630nm. To the best of our knowledge we don't know any further scientific publication dealing with this combination. Despite both devices, the periodic baseline is still required due to the different influencing factors (mentioned by the referee) in both devices, in particular the contamination of the mirror by aerosol particles in the CAPS PMex. The gas monitor can best be used as a reference, e.g. to point out any strong fluctuations of absorbing gases. However, this means that the consideration presented in this article is not obsolete but still relevant.

Due to a lack of literature and the reason mentioned above, we have only slightly changed the article:

"The use of a gas monitor in parallel operation can serve as a reference to adjust the baseline period. However, the new method can be used to take into account a continuous change of the background signal and improve the quality of the resulting extinction values."

Page 2, lines 9/10: The referenced work of Petzold et al., as far as I can ascertain, *only undertook characterisation of a 630nm CAPS PMex unit. It would be worth stating this explicitly, particularly given that the biases in this work are only seen for units operating at wavelengths where the NO2 absorbs strongly.*

We consider the specification of the wavelength of each single cited publication with a CAPS PMex in the context of the introduction as unnecessary. In addition, it is already pointed out several times in the text that the larger deviations occur for 450 and 520nm.

Page 2, line 13: here and throughout the manuscript the paper refers to the gaseous absorption leading to a baseline drift. I think this is confusing. The baseline in these instruments is determined by such quantities as mirror cleanliness, mirror alignment, and near-constant Rayleigh scattering. Over time the baseline may drift due to temperature, ambient pressure changes etc. However, I view the NO2 absorption bias as more akin to a signal measurement. It doesn't drift, but rather is a quantity that varies dynamically and, as shown in the paper, with strong correlation to the particle signal of interest. I would prefer to have separation in terminology for these two distinct causes of error i.e. drift vs gaseous absorber signal.

It's a question of point of view. If deviations from near-constant Rayleigh scattering and/or temperature and pressure influence are attributed to the drift, why not the influence of absorbing gases? The focus of this article are particle extinction monitor (extinction by aerosol particles). Therefore we keep the terminology, although we understand the intentions of the referee.

Section 3: can you explain why the ascending flank is steeper than the descending flank (line 19)?

A possible explanation would be: Traffic peaks as sources arise quickly and directly. Dilution process as a sink is a relative slow process. However, no further data are available for interpretation.

Section 3.2: do the data presented in Figure 3 represent an independent test of the correction scheme. i.e. are the data that were used to tune the scheme the same data that have been plotted in the histograms?

No, maybe it's badly phrased. Just the data points from baseline periods are used as predictor variables. The data points from measurement periods are used for testing. The smoothing parameter are determined by a separate test data set (see previous point above).

Conclusions: I think the conclusions could be seen to provide contradictory guidance to users currently. On the one hand they suggest the new corrections could allow reduced frequency of baseline periods, but on the other suggest users should spend a lot of time filtering in order to characterise backgrounds adequately. I think the paper needs to more clearly describe that, in the absence of scrubbing of gaseous absorbers, users will never do better than having a designated CAPS measuring the gas phase background. If setups have less than this then it could come with cost in terms of residual errors from gaseous absorbers.

Indeed, the last section is really badly phrased and therefore contradictory. However, at this point the consequences resulting from the interpolation should be presented.

The supposedly contradictory statement is a result of the qualitative gain and the limitation of the interpolation

Undisputed, for low variable background conditions (variability is significantly smaller than the baseline period) this approach enable the possibility to reduce the baseline periods. On the other hand, the background variability in the majority of cases is unknown and partially coupled. So, if one considers the background signal as equivalent, the measuring and baseline periods should be equally weighted.

The last section has been rewritten to make it more precise:

" If the change of the background signal is relatively slow, the new method allows to reduce the frequency of baseline periods and thus reduce number of position changes of the built-in ball valve extending its lifetime. On the other hand, in the majority of cases, the background variability and the ambient aerosol and the composition of the carrier gases may be closely coupled (e.g. near traffic emission). From this it follows that the measuring and baseline period should be equally weighted, if one considers the background signal as equivalent. The use of a gas monitor in parallel operation can serve as a reference to adjust the baseline period. However, the new method can be used to take into account a continuous change of the background signal and improve the quality of the resulting extinction values."

Figure 4: the biases described in the bulk of this paper impact measurement accuracy rather than precision. I think the Allan Variance analysis in Figure 4 risks confusing readers with respect to understanding the absolute uncertainty of measurements. For example, it needs to be made clearer than despite the left hand panel of figure 4 suggesting a 1 sigma precision of around 0.1Mm-1, the total measurement uncertainty could be a lot bigger for these measurements.

Also at this point, it seems to be a question of point of view. Of cause, for a single measurement period the effect should be attributed to the accuracy than precision. On a larger time scale, this effect averages out (due to the pos. and neg. deviation, depend-

ing on increasing or decreasing baseline or loss values). This just results in a spread of values, which should be attributed to precision. The text explicitly distinguishes between the averaged results and the maximum deviations (accuracy) achieved.

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