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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Ozone trend profiles in the stratosphere: combining ground-based data over Central Europe to consider uncertainties" *by* Leonie Bernet et al.

Anonymous Referee #2

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1 Short resume

Outlying measurements are a nuisance to many types of analysis. Time series analysis in particular can be very sensitive to outliers, impacting both the estimated regression coefficients and their uncertainty. This topic is especially relevant for ozone profile trend assessments as the actual ozone trend is expected to be quite small (not more than $\sim 2\%$ per decade) which makes robust detection tricky and susceptible to a handful of outliers.

This paper starts off by presenting a comprehensive analysis of periods of outlying

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measurements in the GROMOS time series. Where most other studies stop here and simply reject the outliers from further analysis, the authors apply a regression method proposed by von Clarmann et al (2010) which uses the timing of the detected/suspected outlying data and infers their magnitude along with other components in the regression model, such as the linear trend. Bernet et al. illustrate the value of the method using synthetic data, before applying it to the actual GROMOS time series. The methodology is explained well and the application is very relevant and adequately elaborated.

The last part of the paper moves slightly away from the core subject of the paper, and briefly discusses the impact of sampling and length of the time series on the GROMOS trend result. These are also compared to trends obtained from neighbouring ground-based data records and Aura MLS, however, the adopted outlier detection and incorporation method are not for these data sets.

2 Recommendation

This paper is very well written and the material presented supports the claims made by the authors. The subject is scientifically very relevant and fits the scope of ACP. I would therefore highly recommend to publish this paper as soon as my comments below have been incorporated.

3 Major comments

I ordered major comments in order of appearance in the text.

3.1 Order of vertical regridding and smoothing

p.7, l.7-9: The order of regridding and smoothing is unintuitive. First you downgrade highly resolved vertical profiles to a coarser grid, then convolve these with the MWR averaging kernel and a priori. In reality, the MWR instrument does not vertically smooth a coarse atmosphere. Shouldn't the procedure be the other way around? First smooth at best available vertical resolution, then regrid to the coarse grid. Hence you should oversample the averaging kernel in one direction to match the sampling resolution of the x_h, as in Eqs. 10-11 of Keppens et al. (2015, AMT).

3.2 Unconventional choice of definition relative difference

p.7, l.24: The relative difference is defined as $\Delta = 100 \times (GR - X)/GR$. Why did you not choose $\Delta' = 100 \times (GR - X)/X$, which is the more widely adopted definition? The ratio between both definitions is $\Delta/\Delta' = X/GR \geq 0$ (you removed all negative values; p.6, l.24-25). Your expression will be more sensitive to detect $GR < X$, the conventional expression is more sensitive to detect $GR > X$. Did you test the sensitivity of the detected periods to this definition?

3.3 Description far away from application

The description of the methodology (Sects. 2.2 and 2.3) is quite far away from the actual application. This makes it a slightly more difficult. You could consider explaining the outlier detection and regression methodologies right before their application in Sects. 3 and 4, rather than in Sect. 2.

3.4 Outliers are only detected & considered for GROMOS

You should state clearly that the proposed outlier detection and outlier incorporation methods are only applied to the analysis of the GROMOS time series. You could have done that for the other instruments as well, this would have resulted in a more fair comparison and improved the discussion in Sect. 4.5.

3.5 Show trend results when outliers are removed

Many, if not most, researchers remove outlying data points prior to regression. I am interested in seeing how this simple approach performs in the particular case of real GROMOS data (Sect. 4.2, Fig. 7) and of synthetic data (Sect. 4.1, Fig. 6). I acknowledge that this will not allow to draw conclusions that apply generally, since the result depends on the number and character of the outliers. At least this shows whether it was worth to invest extra coding time and analysis effort.

3.6 Expand discussion to trend uncertainty

The discussion in Sect. 4.1 is very insightful but does not treat another important factor in trend analysis: trend uncertainty. Can you elaborate by how much the outliers affect the trend uncertainty and whether the more advanced method is also able to provide more robust estimates of trend uncertainty?

One element that determines trend uncertainty is the noise in the time series. The example shown in Sect. 4.1 is hence an idealised case without random uncertainties. The few added outliers will therefore have a larger impact on the trend estimate than in the more realistic case where noise would have been present. Have you studied this effect? And please add a comment that the influence of outliers may be smaller in the case random errors would have been simulated as well.

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3.7 Positive trend at lower altitudes?

Please tone down the statement on p.14, l.33-35: "This result implies that ozone might also recover at lower altitudes, but the uncertainties, the dependency on anomalies, and the insignificance of the corrected trend show that this result is less robust." I read it as (1) there is a recovery (2) but the result is less robust. So, do you claim a recovery in this altitude region, or not? In fact, it is the region where GROMOS trends differ most from those obtained by other satellite- and ground-based techniques. Hence, more caution is needed in how this is phrased.

4 Minor comments

p.1, l.0: The title does not convey the main message of the paper. It should be improved so readers will find your work more easily. First, the manuscript is all about detecting unusual observations and taking these into account in the regression. Hence the "to consider uncertainties" is too vague, I believe you should be more specific. Uncertainties can mean anything, really. Second, the presence of "combining ground-based data" suggests that you merged data sets prior to regression, which is not the case. This is misleading, which is definitely undesired for a title of a paper. What about something along the lines of "Combined study of ground-based ozone profile data over Central Europe to detect and incorporate anomalous observations in the analysis of trends in the stratosphere"

p.1, l.1-15: The abstract should be improved, as it is not clear exactly what the paper adds to the existing body of literature. For instance, "[...] an approach for handling suspicious anomalies [...]" does not say how you handle anomalies. This can be done in many ways. In my view, you should state clearly (1) that you analysed multiple ground-based data records to detect anomalous periods in the Bern MWR data record,

and (2) that you then used this information to regress the Bern time series for long-term trends and the temporary bias for the detected anomalous data taking periods.

p.1, l.18: "[...] in recent years [...]". Add LOTUS Report and replace (WMO, 2014) by (WMO, 2018) to the citation. Also, in the submitted version you sometimes refer to (WMO, 2014) and sometimes to (Pawson et al, 2014). Choose just one of these where relevant.

p.2, l.6-8: Incorrect language. The linear trend fitted represents the linear component in the time series after all other natural variations are accounted for (solar, QBO, ENSO, aerosol, ...). This linear term is expected to receive contributions from decreasing ODS and increasing GHG, and possibly other unidentified processes. It is not possible to fit a linear term due to ODS and another linear term due to GHG, since these terms are fully dependent. Hence, it is incorrect to state that "a trend might be masked by natural variability and factors such as GHG increases and changing dynamics". So this needs to be rephrased.

p.2, l.10: Different in what sense? If you combine data records from different instruments, ok. But here such a merging is not considered. So a "changing resolution" or a "changing sampling pattern" is more relevant for a time series composed of measurements by one instrument.

p.2, l.11: Add Frith et al. (2017) to the citation. The paper is more recent but also deals with ozone profiles which is closer to what you report in the manuscript.

p.2, l.12-14: The influence of outliers at start and end points on the trend estimates is well known and not discovered by Bai et al as suggested by the current phrasing. I propose to move the citation to the end of the phrase such as (e.g., Bai et al., 2017).

p.2, l.20: I am not sure there is evidence that all data sets used by Steinbrecht et al. (2017) have been successfully corrected for drift. Hubert et al. reported drift in parts of the HALOE, SCIAMACHY and GOMOS data sets. These have not been corrected.

And so far no one has proven that the OSIRIS correction is removing the entire drift. Please rephrase this sentence.

p.2, l.34: Add a reference to the LOTUS report as it contains the most recent and complete set of trend estimates.

p.3, l.1: Confusing language "handle [...] anomalies by considering anomalies [...]". It would help to define up front what you mean with "anomaly". Is it due to the instrument, due to natural processes, ...? A great deal of readers will read anomaly as something that is not problematic, as it is caused by natural processes. Others will interpret it as an issue to solve.

p.3, l.5: "[...] resulting in a corrected trend estimate [...]". Corrected with respect to what? Perhaps "improved" is more in place here?

p.3, l.12: The word "anomaly" is often also used for anomalous geophysical events. This class of anomalies is not the subject of this manuscript. In caption of Fig. 1 you use "anomaly" in the sense of a "deviation from a climatology", which agrees with how many readers will interpret it. To avoid any confusion I suggest to define "anomaly" unambiguously at the beginning of the manuscript (and perhaps repeated here and there in the text). And are inhomogeneity (see comment below) and anomaly the same for you?

p.3, l.11: Section 2 is a tad long. If you consider trimming the manuscript (which is not what I propose), then this section would be a good place.

p.4, l.16: Add "mean" or "median" to the moving window to clarify what statistical measure you used for the location of the smoothed data.

p.5, l.17: Replace by "[...] using concurrent total column ozone data from the Dobson [...]". This to clarify that the corrections are done using data taken at the same/similar time.

p.6, l.4: You mentioned the spectral line for the ground-based MWR, so it would be

nice to have the frequency of the line for Aura MLS as well.

p.6, l.7: Improve language "stable with insignificant drifts", this is twice the same information. Either use "stable", or more precisely "stable within X% per decade", or just "because there are no drifts between".

p.6, l.9: Clarify what data is compared. E.g. "Comparison of time series". (Further on in the paper there is also a comparison of the trends.)

p.6, l.17: Why is the GROMOS retrieval accurate between 31-0.8 hPa? The retrieval is not accurate simply because the measurement response is high. The instrument can still be biased (large systematic error) and even imprecise (large random uncertainty). The use of "accurate" suggests a small uncertainty. Is that really the case?

p.6, l.22-24: The native measurement coordinate system for lidar is number density versus altitude. You need to explain how the lidar data are converted as well. For ozonesonde this is trivial due to the temperature data from the attached radiosonde.

p.6, l.26-29: Please clarify the details of the regridding procedure. The description is confusing and I am not sure I understand the order of operations and on what observed quantities.

p.6, l.26-29: Also, is the interpolation a simple linear interpolation or is it a more advanced method such as described in Calisesi et al. (2005)?

p.7, l.3 and p.7, l.21: Remove "direct" from "direct comparison", since there are no indirect comparisons in this manuscript.

p.7, l.25-27: The use of "corrected" relative difference is misleading. Why not e.g. "debiased" relative difference or "variations of the" relative difference? You simply remove the mean level to look at deviations of the relative difference w.r.t. its mean level. Please abstain from using "corrected relative difference" elsewhere in the text as well.

p.7, l.25-27: Add formula to clarify that you remove a constant offset in RD. In other

words, assuming RD_i is the monthly mean of month i and the mean of RD over all months is μ_{RD}, then you debiased the RD time series using $RD_i - \mu_{RD}$.

p.8, l.19-20: Von Clarmann present an approach to consider "known", "identified" or "suspected" inhomogeneities in the trend analysis. Their method does not identify the time of an inhomogeneity, but co-fits the magnitude of the temporal offset. Second remark, state right here that you apply the von Clarmann method and code.

p.8, l.15-...: Now you start to use "inhomogeneities" rather than "anomalies". Is there a difference between these terms? Please define these clearly, if they are. If not, then state that as well.

p.8., l.15: Strengthen the link with previous Section 2.2. State asap that you will now use the times of the anomalies detected by the previously described method (Sect. 2.2) in the regression scheme (Sect. 2.3).

p.8, l.15-16 and/or l.23-24: Clarify that the full error covariance matrix describes the correlation between measurements, not between pressure levels.

p.8, l.21-22: Remove the entire phrase "Another reason for [...]". Instead add this possible cause (unknown origin) to the end of the phrase on l.16-18 "Inhomogeneous data can originate from [...] spatial or temporal sampling." (which currently lists known causes). The method you described in Sect 2.2 identifies periods of anomalies, but does not identify the cause of the anomaly. It can be anything in the list of l.16-18, but also unknown instrumental issues.

p.9, l.5: "no error correlation", but in what domain? Clarify that you deal with the correlation between measurements, not between pressure levels.

p.9, l.5: You introduce a second VCM (variance-covariance matrix). It would help to have a separate symbol for the different VCM's (S_1, S_2, S_{instr},$S_{autocorr}$ or whatever) and use in-line formulas to explain when you add these and when not. This allows you to get away from unclear language such as "additional covariance matrix" and

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"enhanced covariance matrix". You could just refer to it as $S' = S_1 + S_2$. This also

p.9, l.12: Clarify "which means the time correlated residuals" are not considered (S_2 or $S_{autocorr}$).

p.9, l.15: Now you switch back to using "anomalies", not "inhomogeneities". Be consistent or mention that both terms have identical meaning.

p.9, l.16: It is important to link with previous section. "[...] for months where anomalies were identified (using the method described in Sect. 2.2)".

p.9, l.18: Are you using the so-called "corrected relative differences" or not?

p.9, l.24: Replace "low" values by "small" values. E.g. -25% is a very low value, but not a small value when compared to -5%. I know the example is not applicable here, but I would generally suggest to refrain from using "low/high" and use "small/large" instead when referring to the magnitude of values (not the sign).

p.9, l.29: Clearly state that above procedure is only applied to GROMOS data. You did not consider outliers in any other time series than GROMOS.

p.9, l.32-34: The percentage trend is obtained by dividing the ppmv trend by the mean level. If there is a trend the mean value will depend on the period over which the mean is computed. Did you use exactly same period for all trends? Since Aura/MLS has the shortest record, I would guess the ppmv trend should be scaled to 2005-2017 mean values. Has this been done? If not, please state whether this effect is negligible.

p.10, l.1: You could remove ", as described by Tiao et al. (1990)", as this is just introductory-level Gaussian statistics.

p.11, l.1-2: You refer to "another temporal sampling", another than the other instruments? Another than the usual GROMOS sampling?

p.11, l.9-10: Remove ambiguity. You deal with relative differences of monthly mean values of time coincident pairs, not of the monthly mean value of the relative difference

of time coincident pairs. Figure 3 suggests the latter however.

p.11, l.15-17: The large outliers in the OHP comparison time series (Fig. 3) are all negative. The explanation is not satisfying, if not incorrect. If outliers are due to the small sample, then large positive peaks should be observed as well. Unless there is a systematic component in both the sampling pattern and the ozone fields. The latter seems highly unlikely to me. Can't it, instead, be due to the presence of large positive outliers in the OHP ozonesonde record?

p.11, l.9: Does Fig. 3 show the "corrected relative difference"? I guess not, since the mean level seems to differ from zero. This should be clarified.

p.11, l.21: Doesn't Fig. 4 show the "corrected relative difference" (or debiased relative difference, see earlier comment above)? Mention this clearly in the text, and abstain from using "corrected relative difference", I like "debiased relative difference" better.

p.11, l.34: Replace by "[...] comparing GROMOS to SOMORA [....]". There is only one reference instrument in the US during the period before Aura/MLS.

p.12, l.1: Add "[...] at these altitudes, especially prior to the start of the MLS measurements in 2004." And you could then e.g. also mention the step change around 2005 visible in panel (a) around 2005 which may be related to the change of SOMORA front end (see also comment below; p.28, Fig.3).

p.12, l-7.8: It is not entirely clear whether you are saying here that you disprove the claim by Steinbrecht (2009)? If yes, then end the phrase by removing the ambiguity. For instance: "[...] due to instrumental issues of GROMOS and not due to sampling."

p.12, l.7-8: Are there any leads on what could be the cause of the instrumental issues? If yes, it may be of interest to the reader.

p.12, l.21: A negative amplitude has no meaning. Is this a typo?

p.12, l.26: Vague language "This might be due to some error propagation". This clause

does not hold additional information and may as well be removed.

p.13, l.4: You arbitrarily chose 5%, which is $3.5 = 5/(0.1/7)$ times larger than $1.4\% = 0.1/7$. What if you increase to even higher uncertainties, e.g. in the limit of infinite uncertainty? This case would be equivalent to removing the anomaly from the time series prior to regression. (See also my major comment)

p.13, l.6: Text is inconsistent with caption of Fig. 6. Shouldn't it be "[...] once without (case D) and once with (case E) the increased [...]"?

p.13, l.7: Add to the last phrase that a 5 ppm correlated block essentially leads to a free fit of the magnitude bias.

p.13, l.27: Repeat by how much you increased the uncertainty, so a reader does not have to go back all the way to Sect 2.3.

p.13, l.34: "[...] decreases the trend slightly in the lower stratosphere, but the differences are small." Doesn't this point to a too small scaling of the uncertainties?

p.14, l.4: I still don't like the phrasing "corrected" trend profile. Corrected w.r.t. what? See also my comment p.3, l.5.

p.14, l.4 and l.30-31: "The corrected trend profile agrees well with recent satellite-based ozone trends [...]". I am not convinced that the case III results agree well with other studies. They are consistent with Steinbrecht (2017; Fig.5, Table 6) between 10–2 hPa (what you call "middle" stratosphere). However, there is tension between the results at 30-10 hPa ("lower" stratosphere). The other studies find smaller trend values, more closely to 0–1% per decade.

p.14, l.13-14: Somewhat confusing phrasing "a slight shift in the peak height". A shift with respect to what? Is the peak shifting in time, which is what I first think of in the context of time series analysis? More likely you mean that the peak sensitivity of the GROMOS retrievals is not at the true altitude?

p.14, l.30-31: See earlier comment, I would refrain from using "agree". The results are consistent, but do not agree well especially below the 10 hPa level. The bias corrected trend does lead to a better agreement

p.15, l.16: Unlike Reviewer 1, I like the fact that the full altitude range is shown. This section is not about a comparison to actual ozonesonde or lidar trends, but about the impact of sampling on GROMOS trends. I would keep the altitude range in Fig. 8 as is.

p.15, l.17-19: This is a very nice piece of information. Out of curiosity, have you tested to randomly subsample the GROMOS time series to N_{MOH} and N_{Pay}, then regress? Such an analysis would add information about the random nature of the impact of sampling. The more positive sonde trend at 3 hPa may as well turn into a less positive trend if another temporal GROMOS sampling was picked but with same sample size as the ozonesonde time series. Would be nice, but not necessary.

p.15, l.26: Replace "estimations" by "regression".

p.15, l.26-27: Did you average the GROMOS trends or the GROMOS time series? If the former, how did you do that and does the trend of vertically averaged data agree with the vertical average of the trends?

p.16, l.5-6: Vague language "The trend dependency [...] is controversial to [...]". Please rephrase, I do not understand what you mean.

p.16, l.6-7: "This suggests that the true trend might not be linear, or that some interannual variations or anomalies are not captured by the trend model" This is known for a long time. Please rephrase to "This illustrates that [...]".

p.17, l.2-3: "A thorough harmonization would be necessary to correct the trend for this change." In fact, your manuscript describes a method that does not require harmonisation. I understand the extra work effort, but it is a pity for Section 4.5 that you did not treat outlying data in the non-GROMOS regression analyses. This would have made an even more interesting comparison.

p.17, l.4: It is unclear whether you have used these newer SOMORA retrievals or not. Please clarify in the revised manuscript.

p.26, Fig.1: "[...] indicate months without data." Missing data does not imply there are no data, and you mean there are no (screened) data during these months.

p.26, Fig.1: Mention the period over which the climatology is computed. So, "Deviation from GROMOS monthly mean 1997-2017 climatology" would make a better description.

p.28, Fig.3: "Monthly means of relative differences" implies you compute relative difference $100 \times (GR - X)/GR$ for each coincident pair, then take the monthly average. This is not how you described it in Sect. 2.2.

p.28, Fig.3: Do these time series represent the "relative difference" or the "corrected relative difference"? If these are corrected relative differences, then how can it be that most curves seem to have a negative mean value where zero would be expected?

p.28; Fig.3: Panel (a) shows a step around 2004–2006. Is this due to the change of front end in SOMORA in 2005 (p.4, l.21)? If yes, then it would be nice to at least mention this in the last paragraph of p.11.

p.29, Fig.4: Do all panels represent the "relative difference" or the "corrected relative difference"? Clarify in the caption in the latter case.

p.34, Fig.9: See my earlier comment. Did you average the trend, or average the time series then derive the trend? In the first case, how exactly did you compute the error on averaged trend?

p.34, Fig.9: Mention significance level of the error bars. I assume that these represent 1σ since some bars that do not cross the zero level are greyed out.

p.37, Table.2: Add time unit in first column. It should be "ppm/decade".

p.37, Table.2: Move third column ("Monthly uncert.") to first column in section "Param-

eters in the trend programme". No uncertainty has been added in the time series.

p.37, Table.2: Use consistent number of significant digits. I suggest three digits for all numbers quoted.

5 Technical corrections

p.1, l.4-5: Replace by "[...] anomalies that may all mask a [...]".

p.1, l.7: Remove "[...] to improve the derived trend profiles [...]". This is evident.

p.1, l.11: Replace by "[...] in agreement with satellite [...]".

p.1, l.17: What is a "serious" decrease? Perhaps "fast" or "large" is more appropriate language?

p.1, l.20: Replace by "[...] Antarctic ozone concentrations started [...]".

p.2, l.1: Replace by "[...] increasing ozone levels are more difficult [...]".

p.2, l.1: Replace by "[...] to detect and these depend on altitude [...]".

p.2, l.7: Add "s" to "[...] greenhouse gas increases [...]".

p.2, l.19-20: Replace by "[...] with no or small drifts [...]".

p.2, l.25: Remove "data" from "[...] data steps [...]".

p.2, l.27: Move the "yet" to "[...] has not yet been [...]".

p.3, l.21: Replace by "[...] They measure the 142 GHz line where ozone molecules [...]". Currently you have "[..] atmospheric emission [...] molecules emit [...]".

p.3, l.29: Replace by "[...] is the main focus [...]".

p.4, l.10: Replace "instead" by "rather than from".

p.4, l.12: "data corrections".

p.4, l.13: "troposphere" is possibly more precise terminology here, rather than "atmosphere"? This then also links better with next phrase which contains "tropospheric humidity".

p.4, l.16: "[...] 3-day moving [...]". Drop "s".

p.4, l.18: Replace by "[...] outliers exceeding four times [...]".

p.4, l.18: "[...] 30-day moving [...]". Drop "s".

p.4, l.34: Move the last phrase "The lidar can only [...] the influence of sunlight." to the first paragraph of Sect. 2.1.2. This to avoid confusion that this information holds for all lidars, not just the one installed at Hohenpeissenberg which is the subject of this paragraph.

p.5, l.9: Remove newline, and ensure the phrase "More detailed information [...]" is next to the one ending in "[...] with the GROMOS limits." Since the phrase only contains information for OHP.

p.5, l.28: Replace by "[...] 30 km, above which the balloon [...]". The balloon does not usually burst at "30 km", but at "30 km or above".

p.6, l.2: Replace by "[...] Aura satellite, launched in mid 2004, [...]".

p.7, l.4: Replace by "The vertical resolution of GROMOS and SOMORA are usually coarser than for the other instruments. [...]".

p.7, l.17: Replace by "[...] GROMOS and SOMORA have a higher temporal resolution than the other instruments. [...]".

p.8, l.18: "temporally correlated".

p.8, l.22: Remove "that lead to anomalies". Otherwise "[...] reason for inhomogeneities might be [...] issues that lead to anomalies [...]".

p.9, l.7: Replace "adjusted" by "scaled", because that is what you do.

p.9, l.8: Replace by "[...] the trend fit becomes unity."

p.9, l.20: Some irrelevant information. Replace by "[...] In a second step, we account for biases [...]".

p.9, l.27: Drop "have" from "we have found".

p.9, l.31: Remove "and the Aura/MLS trend starts in Jan. 2005", as this is duplicated in the next phrase.

p.9, l.32: Replace by "Aura/MLS cover the shortest trend period, starting in [...]".

p.9, l.33: Add "regression" to "regression model output", to avoid any confusion with e.g. CCM's.

p.10, l.28: Replace altitude "classes" by "ranges".

p.11, l.1: "[...] whereas the GROMOS data shown here [...]".

p.12, l.20: Replace by "[...] per decade, i.e. $b = 0.1$ [...]".

p.12, l.25-26: Replace by "The residuals are of order 10^{-6} and increase towards the start and end of the time series (Fig. 5(b))."

p.13, l.12-13: Rephrase, it is hard to read. "We further found that the trend estimate is closer to its true value when higher uncertainties are chosen [...]".

p.14, l.11: Replace by "[...] even though the GROMOS [...]".

p.16, l.22: How do lidar data "derive" from satellite data? Did you mean "deviate", perhaps?

p.17, l.29: Replace by "[...] in the trend analysis [...]".

p.26, Fig. 1: Not "stripes" but "lines".

p.32, Fig.7: Remove the space before "case II" in the parenthesis on the second line of the caption.

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