Response to Referee #1

(***Referee report**: https://doi.org/10.5194/amt-2023-28-RC1*)

Manuscript:

Innerkofler, J., Kirchengast, G., Schwärz, M., Marquardt, C., and Andres, Y.: *GNSS radio occultation excess phase processing for climate applications including uncertainty estimation*, Atmos. Meas. Tech. Discuss. [preprint], https://doi.org/10.5194/amt-2023-28, in review, 2023.

The authors thank the reviewer very much for the constructive and detailed feedback to the manuscript. We thoroughly considered all comments and carefully revised the manuscript accounting for them. Below are our point-by-point responses.

Comments by the reviewer are cited black upright, our responses are red. Line numbers used in our responses refer to the original AMT Discussions paper and text updates in the revised manuscript are quoted below in blue)

All citations referenced are provided in the revised manuscript.

Summary

The authors present a detailed and valuable summary of the rOPS L1a excess phase processing system that includes excess phase uncertainty estimation. The detailed processing description is well done. The uncertainty estimate portion of the paper should be updated to address the questions/comments below.

One aspect that the paper does not include and should, that would improve it, would be to include a discussion in the intro of how the uncertainty estimates described here would be used to improve the quality of the final ECVs. Are these uncertainties being used now to better derive BA, N, ...? Or will they only be propagated to higher level to provide uncertainty estimates of the ECVs? What about vertically correlated phase errors, or phase rates, due to LEO orbits, GNSS clocks or ionosphere residuals? Are they taken into account? These correlations will lead to larger errors for ECVs when integrated downward with the Abel inversion.

The subsequent usage of the estimated uncertainties at excess phase level and their impact on the quality of the following processing is discussed in the references provided at L69-L73. The uncertainties are used in the upper boundary initialization (statistical optimization) of bending angles before the refractivity retrieval as well as in the moist air profiles retrieval as part of the backgroud information (in the 1DVar/optimal estimation). We added the following paragraph to provide the reader with this information and advise how uncertainties are handled within the subsequent retrieval chain:

The random and systematic uncertainty estimates at excess phase level are then propagated through the entire ODP retrieval chain in order to provide the final ECVs with their associated uncertainties. Additionally, the uncertainties quantified are employed in part of the retrieval operators of rOPS to improve the derivation of variables (e.g., ionosphere correction, statistical optimization, moist air retrieval). For details on the uncertainty propagation along this chain, starting from the estimates at excess phase level, see Schwarz et al. (2018, 2017); Schwarz (2018); Li et al. (2019).

Another concern is the 3 data periods used in the study – they do not cover the most challenging regimes that RO has to track in. Analyzing a more challenging period may shed more light on RO error sources and uncertainty and better inform the community.

Regarding the selection of the test data periods comments are provided below (first comment under “Detailed Questions/Comments”).

I believe this paper is a valuable contribution to RO and climate research and should be published with minor revisions.

The authors thank the reviewer very much for the valuable comments that helped to significantly improve the manuscript.

Details Questions/Comments

L121: 3 3-month time periods:

- 2008 (Jul-Sep), solar min
- 2013 (Jul-Sep), solar max, but not in Equatorial plasma bubble scintillation season
- 2019-20 (Dec-Feb), solar min

These 3 periods do not present the strongest challenge for RO data processing, quality control, and uncertainty evaluation. Solar max periods during Sept-March present the greatest challenge for RO especially in the equatorial region. This paper would provide a better understanding of RO uncertainty and issues if it included the most challenging conditions for RO during solar max and Fall-spring periods. If the authors can’t include analysis of these data, then they should at least discuss any issues seen in these more challenging data.

Thank you for pointing towards the more challenging test period in the 2013 equatorial plasma bubble season for the propagation of radio signals. After careful consideration however, we came to the conclusion that the test data periods chosen serve the demonstrative purpose of this introductory paper of the L1a excess phase processing including uncertainty estimation and that reprocessing would be beyond the scope of this purpose. However, we will keep the referee’s comment regarding the special case of equatorial plasma bubble season in mind for follow-up evaluations.

L146: ERA5 analysis used for validation of RO profiles. This validation is tricky, since ERA5 analysis already assimilates the RO profiles.

Yes, as stated in L150, the ERA5 analysis assimilates observational data including RO measurements. In this study the use of the ERA5 analysis data is limited to the sensitivity analysis performed in Section 4.1.1. For the task of pure assessment of the quality and stability of the implemented excess phase processing we consider this sufficient, although we are aware that the assimilation of RO data has an influence on the analysis (e.g., Schmidt, 2008). For genuine validation studies, the use of independent datasets is clearly advisable, in addition to the use of the ERA5 analysis data. We added a change as follows:

"… while the ERA5 analysis data are used for the provision of reference profiles in part of the sensitivity analysis of the RO retrieval."

L152: use suit, not suite

Thank you, the typo has been corrected in the manuscript.

L164: What if you don't have the GNSS navigation bits from the ground network? Do you process it anyway?

If GNSS navigation bit data are not available from the ground network we apply an internal removal by detection of phase switches between adjacent samples. Therefore, we process the data in any case. A more detailed description of navigation bit handling is provided in the paragraph starting at L423.

L175: use builds, not builts

Thank you, corrected in the manuscript.

L181: use pseudo-range, not pseudocode

Thank you, corrected in the manuscript.

L185: Can you provide some information in the text about the magnitudes of the computed systematic and random orbit uncertainties?

The following information regarding the estimated orbit uncertainties from the precise orbit determination is now provided in the revised manuscript:

"In general, the combined-3D position and velocity uncertainties estimates for the Metop satellite series amount to about 1.9 cm and 0.02 mm/s (for random) and 5.0 cm and 0.05 mm/s (for systematic), respectively."

L200: Table 2, should the units of GNSS clock bias be seconds (not m)?

Yes correct; changed in the manuscript.

L242: Does the linear combination of L1 and L2 phase at the same time result in over estimation of uncertainty. I assume it does since the L1 and L2 ray paths are different.

In the estimation of the uncertainty the linearly-combined excess phase profile LC from of L1 and L2 data includes ionospheric residuals, while the modeled excess phase is based on the neutral gas atmosphere without consideration of ionospheric influences. This leads to a conservative estimation of the uncertainty, as assumed by the reviewer. The LC excess phase profile here is only used for auxiliary information; in the state retrieval, the ionosphere correction takes place at bending angle level (as described in Schwarz et al., 2018).

L270: Q: how good is your model excess phase profile? Why not raytrace through ERA5 to get the model excess phase profile? I guess this won't work in the lower troposphere, but I doubt the excess phase data in the LT are very useful. You could at least validate your model excess phase above the LT where signal is small with the raytracing excess phase.

Evaluation with raytracing showed that the difference is very small, apart from the lower troposphere (where still the relative difference to data is very small; see, e.g., Schwarz et al., 2018; Appendix example therein on time series filtering based on the delta-signal upon subtracting the modeled excess phase).

L304: use, occultations that may miss ….

Thank you, changed in the manuscript.

L310-315: One disadvantage of the GRAS OL approach that should be mentioned here is that since it must track the CA code, it loses lock when the CA signal gets too noisy in the LT which results in some data gaps. Data gaps are bad for RO and can break SI-traceability of the observations. What do you do about data gaps?

In order to minimize the effect of data gaps on the SI-traceability of the observations, we analyze the measured data segments per individual occultation event and treat them following recommendations of the data provider as follows. We select the longest continuous closed-loop (CL) and raw-sampling (RS) data segments not allowing sampling-time deviations within these segments to be larger than 5 % of the nominal sampling time stamps. The RS data are then down-sampled to 50 Hz and termed open-loop (OL) data thereafter. The two selected CL and OL data segments are usually overlapping or adjacent. When combining the CL and OL data we dismissed the OL if there was any gap between the two data segments. This accordingly reduces the tropospheric penetration depth for those specific occultation events. In the latest implementation of the rOPS, following the data provider recommendations, a maximum gap of 1.2 s between CL and OL is allowed, which is bridged by linear interpolation. SI-traceability is somewhat degraded by how efficient the data gaps are connected. We noted this in the manuscript as follows:

"This can lead to data gaps when the C/A code tracking loses lock caused by challenging tracking conditions in the lower troposphere (Schreiner et al., 2011). Therefore, in order not to degrade SI-traceability, we restrict the processed data to the longest continuous CL and RS data segments not allowing any gaps between these two data segments. Another … "

L359: remove 'most'. I don't think most RO missions use USO's like Metop, i.e., C-1, Spire, Champ, Kompsat-5, ..

Since there are quite a few RO missions besides Metop who use USOs (e.g., GRACE, FY-3, C-2) we rephrased the sentence accordingly.

"However, among other RO missions, Metop-A/B/C use ultra-stable quartz oscillators that are likewise highly accurate over the short term of RO events."

L461: A problem with this is that if you apply a conservative QC before uncertainty estimation, your uncertainty estimates will be under-estimated. Can you add some discussion on how you came up with the proper QC to obtain reliable uncertainty estimates?

In general, we aim to only exclude un-physical profiles from the subsequent uncertainty estimation and the subsequent ODP-retrieval, in order to facilitate properly estimated uncertainty (without influence of illegitimate outlier data). This is also done in order to ensure inclusion of all reasonable profiles for rigorous climate processing.

L465-470: Figure 7, is the BB, just the LC – FMO?

Also, Fig7 right panel, shouldn't the HPBB have the high frequency variations, and the LPBB have the low frequency variations?

Exactly the BB is LC - FMO, this is also described in more detail in lines 484 – 487. The HFBB actually is the difference between BB and LFBB (cf. line 495), which reduces the high-frequency variations of HFBB compared to LFBB.

L477: use, shorter weak signal

Thank you, changed in the manuscript.

L517: If an outlier is detected, do you remove it so there is a gap in the data, or do you replace it with an interpolated value? Also, what if your model profile is far from truth, how can you be sure you are not removing accurate data? If you remove outliers and create gaps, how can you be sure that you maintain SI-traceability throughout the profile?

Within the level 1a excess phase processing outliers are only detected. Later they are (statistically) corrected in the level 1b bending angle retrieval (with adjusted uncertainties). Using a statistically sound method for the outlier detection algorithm reduces the chance of removing accurate data. For this reason, and in order to maintain SI-traceability, outliers are corrected following this statistical approach in order to prevent data gaps. If an outlier is detected then it is replaced by a normally distributed random number drawn within a $\pm 3\sigma$ standard deviation range. It is hence an adequate fill value not distorting the statistics.

L525: What happens with the outlier detection when there is a cycle slip? L1 or L2? A cycle slip will look like a step in the BB excess phase. Also, it is assumed that occultations with large small-scale ionosphere residuals are captured with your QC algorithm. Which QC check best catches these ionospherically disturbed profiles? You showed combined QC %'s for all 3 data periods. Did you notice any differences in the QC %'s for the 3 different data periods? I would expect there to be a higher percentage of QC'd profiles for the solar max period.

Will have to do a separated calculation of the percentages for the different periods to answer this question.

The outlier detection checks only within the altitude range, where the altitude mapping of the forward modeling has converged. If a cycle slip occurs within this altitude range (and has not been corrected within the cycle slip detection algorithm before) the resulting step might cause the profile to be flagged (falsely) accordingly. Actually, classical scintillations are too small to be captured in the QC. We recalculated the QC rejection rates for the 3 different data periods and could not find major differences between the periods in 2008, 2013, and 2020.

L563: use, sampling rate along the vertical profile.

Thank you, changed in the manuscript.

L573: I don't see S/C attitude uncertainty included in the uncertainty equation. Every SC has attitude jitter. What is performance of Metop SC? Effect is smaller for larger SC, but it should be mentioned.

This is so far not considered in the uncertainty budget, since the attitude correction is not yet implemented for Metop in our system. After successful verification of the attitude correction, we will address the accompanied uncertainty in more detail. We added the following sentence to the revised manuscript:

"Not yet taken into account is the spacecraft's attitude uncertainty, which will be addressed in more detail once the attitude correction in rOPS is included and verified. For larger spacecrafts like the Metop satellites this effect caused by attitude jitter is expected to be small, however."

L612: I don't understand this, 'carrier wave cycles in order of several cm.' Cycle slips can occur at ½ to N cycles, and therefore can be much larger than several cm.

The authors were referring to "an" undetected cycle slip, which is now corrected in the revised version of the manuscript:

"However, an undetected cycle slip can introduce a phase shift of half or full carrier wave cycles in order of a several centimeters, ..."

L617: I don't understand c = 0.001 m/min? So does this mean you apply an uncertainty due to cycle slips of 2 mm over a 2-min occultation event? This would be too small. Please explain.

We re-checked technical Metop documentation for a more reliable quantitative estimate. We did not come over a clear quantitative estimate but agree that the current setting was clearly too small. We now try to better reflect the effect by adopting a more plausible change of 1 mm/s, i.e., reflecting a 1% slip fraction per second relative to the half-cycle length (about 10 cm), more consistent with the documentation.

Therefore, to account for these undetected cycle slips as an estimated basic uncertainty, we include a change-rate factor *c* = 1 mm/s, reflecting a 1% slip fraction per second relative to the half-cycle length. This leads to a gradual excess phase decrease (cumulative negative bias) with decreasing altitude from the time of highest altitude t_{top}^{DLL} to lowest t_{bot}^{DLL} in DLL measurement mode:

L619: use, Local spacecraft multipath.

We updated the manuscript accordingly.

This description of local sc mp is not very well substantiated. First of all, the period of local sc mp on orbit will be closer to the orbital period of 100 min. Also, the amplitude of the effect is related to the geometry of the antenna on the LEO sc and to surface property of the reflecting surface. We found with rough calculation that this effect can result in a phase error rate of close to 0.1 mm/s for a strong reflector. Since the geometry on the sc is fixed, these error may manifest as a basic systematic phase rate error that may not cancel in a climate study using an ensemble of occultations. This 'basic systematic phase rate error' aspect of local sc mp should be mentioned in the text.

Here, we model the effect of local spacecraft multipath during an occultation event (1-2 minutes duration), not to be confused with longer period orbital effects. We classify this effect as apparent systematic uncertainty since with a changing viewing geometry from occultation to occultation the local multipath errors will average down when regional and temporal averages are calculated (Kursinski et al., 1997). The manuscript now includes previous studies using the corresponding model following GRAS specifications with a phase error rate of about 0.05 mm/s (Carrascosa-Sanz et al., 2003):

"The residual local multipath error effects on the phase measurements are modeled using a sinusoidal model, for representative broad beam antennas used in GNSS RO (Steiner and Kirchengast, 2005; Ramsauer and Kirchengast, 2001; Syndergaard, 1999). The sinusoidal shaped function is defined with a multipath phase error amplitude of 0.5 mm and period set to 60 seconds, resulting in multipath errors up to 1 mm, following GRAS-type error specifications (Carrascosa-Sanz et al., 2003). We classify this effect as apparent systematic uncertainty since with a changing viewing geometry from occultation to occultation the local spacecraft multipath errors will average down when regional and temporal averages are calculated (Kursinski et al., 1997)."

L622: Has this statement, 'can be reduced by modelling', been demonstrated experimentally for phase multipath on LEOs? 'The possible phase shifts of up to a few centimeters, introduced by local multipath, can be reduced by modeling the effect and the use of directional antennas'

The current statement was replaced and updated as follows:

"The possible phase shifts of up to a few centimeters, introduced by local spacecraft multipath, can be reduced by proper platform design and the use of directional antennas."

L627: The amplitude of 0.5mm used here seems incredibly small, and the period is much too small. The authors should provide a better justification for numbers or provide references.

For the Metop mission a dedicated effort was undertaken to diminish the effect of strong reflections and therefore a reduced amplitude is assumed. See also the comments above.

Figure 8: caption says thick orange line, but it is blue in the figure.

Fig8: Can you also include daily mean values (different color) in addition to daily median values? This will give some additional information on the impact of outliers.

Figure 8 now includes daily mean values (red) showing modest deviations compared to the daily median values (blue). The figure caption was corrected and updated accordingly.

L654: use, 'on average'

Thank you, changed in the manuscript.

L655: why do the Metop counts get smaller for the later missions?

The decrease in the number of profile counts are due to missing closed loop observations in the input data. We added the following declaration to the revised manuscript:

“Overall, on average, the daily number of profiles amounts to 647 profiles (Metop-A), 610 profiles (Metop-B), and 559 profiles (Metop-C). In the later 2020-JAS period EUMETSAT input data contains files with missing closed loop (either L2 or both frequencies), which reduces the number of processed event in this later study period.”

L675-679 and Fig 10: It appears that the solar max period of 2013 has larger differences for all altitude regimes, as expected due to larger iono residuals. Is this statistically significant? This deserves some discussion from the authors in the text since ionospheric residuals are one of the largest challenges for RO especially at higher altitudes.

Although larger standard deviations can be observed in 2013 period, the box-whiskers in Figure 10 depicting the median (mid-line) and 16 % and 84 % percentile, the zero-line is still within +/- sigma and therefore not supporting the statistical significance. However, comparison against other solar max periods will be of interest in future, in order to learn more about the influence of ionospheric disturbances at excess phase level.

L686: Table 5, why do the orbit differences increase for the later 2020 period? Also, how do you go from the results in Table 5 to specifying the orbit velocity uncertainty above on L604, 0.02 mm/s? 0.02 mm/s seems too small for specifying the orbit velocity uncertainty.

The results in Table 5 represent inter-center differences of orbit solutions based on different software, parametrization, models, and input data, so including additional structural uncertainties, which are not represented in the orbit velocity uncertainty quantified in L604. We understand that the increase of the orbit differences in the later 2020 period is related to differences in the input data used. In the earlier 2013 period reprocessed GNSS orbit and clock data from CODE (repro2015; https://dx.doi.org/10.7892/boris.80011) of higher quality served as input for the precise orbit determination at WEGC, while in 2020 CODE final products (https://dx.doi.org/10.7892/boris.75876.4) were used. Additionally, in 2020-DJF the navigation tracking data from the GRAS zenith antenna were only available as hourly orbit dumps. The pre-processing and merge to a daily input file for the precise orbit determination somewhat diminish the quality further.

L692: Figure 11. How are the excess phase differences computed that are used to generate the stats in the figure? Are they the rms over the altitude region of interest? The maximum difference? Please state in text.

The statistics for each individual layer is calculated by averaging (mean) of the correspondent statistical measure used in the boxplot of Figure 11. We added the following text to L661:

"… layer averages (calculated from the vertical statistical measures, i.e., mean, median, stddev, percentiles, by obtaining the average over all values within the corresponding altitude layer):"

L763: How do the inter-center excess phase differences compare to your previously estimated excess phase errors? It looks like the inter-center differences are much larger than the earlier estimated uncertainties? Are these just due to mismatching (time/space) atmospheric differences? The estimates should be close to the inter-center differences. The authors should include more detailed discussion of the comparison between your estimated uncertainties and the inter-center differences.

In this study we aim for an uncertainty estimation of the observational data; the inter-comparison of excess phase data from different processing centers might include additional structural uncertainties due to the different processing schemes not captured in the uncertainty budget. In particular, the larger deviation of UCAR data in the lower troposphere indicates representation uncertainties from until yet unknown sources. The authors believe that the characteristics of the differences indicate an issue in the processing in the transition of closed loop and open loop measurements. To reassure this assumption. further research will be needed which could be a valuable future task within a broader inter-center comparison (similar to what, e.g., Steiner et al. (2020) did along the retrieval step from bending angle to atmospheric profiles retrieval).

We note that the results from the inter-comparison between excess phase data processed by EUMETSAT, WEGC, and UCAR experience larger differences in the lower troposphere than we quantified in the uncertainty budget. This indicates additional structural uncertainties arising from different processing schemes not captured in the estimated uncertainties of the observational data. In order to address this substantial differences a broader inter-center comparison study is advised.

L775: use, as a synthesis result.

Thank you, changed in the manuscript.

L782: Fig 16, Why is there no kink in the curve between SLTPA of -20 and -40 for the 2008 period, and there is a kink for the later periods? The authors should discuss this clear difference in the text.

We interpret this to originate in the different number of profiles as a function of altitude (Fig. 13), which possibly occurs due to changes in the on-board tracking and OL/CL transition handling of Metop within the different study periods. We added an explanation as follows:

"However, between an SLTP altitude of -20 km and -40 km, the two later periods exhibit a slight kink in the estimated random uncertainty compared to the 2008 period. This is presumably connected to the different structure of the corresponding numbers of profiles as a function of altitude shown in the lower panel of Figure 13 and changes in the receiver tracking."