

Hase Phase Correction Review

General Comments.

This is a very good paper describing a new method of phase correction, which is an important step in the processing of FTIR interferogram data into spectra. Inadequately performed phase correction can cause serious artifacts in the resulting spectra, leading to degraded accuracy of the atmospheric gas amounts retrieved from them, especially in spectral regions containing blacked-out absorption lines. As the accuracy required for atmospheric gas measurements gets more and more stringent, it is very timely that the phase correction process be re-examined and upgraded.

The paper has very high standard of English, especially considering that the authors are all non-native English speakers. I only found a handful of instances where the text needed slight adjustments.

Paper contains too much material describing Bruker spectrometers and the Izana site. This interrupts the thread of the science discussion. Individual instances are cited below in the Specific Comments section below.

Paper ends rather abruptly, with no discussion of the impact on retrieved $x\text{CO}_2$ of the new phase correction for the Vertex or IFS125 spectrometers.

“phase unwrapping” is mentioned in the Abstract and Introduction, but I found no further discussion of this topic.

The effect of the improved phase correction algorithm is very small, at least in the CO_2 bands used by TCCON/COCCON at 6160 to 6380 cm^{-1} , but this window rarely saturates. Perhaps the authors should also investigate a spectral window that contains saturated spectral features close to absorption lines of interest (e.g. HF at 4039 cm^{-1} , CO at 4233 or 4290 cm^{-1}) since it is under these partially saturated conditions where the new algorithm is supposedly most beneficial. I think that it is a serious omission for the paper not to have investigated some more adverse fitting windows, in which the advantages of the new method would be more apparent.

Specific/Technical Comments (Authors' words in black. My comments in blue.)

Lines 30-33: The word “shortly” usually connotes time, in which context it means “soon”. So, I suggest changing sentence to: “Fourier Transform Spectrometry is an important technique for remote observation of atmospheric composition, especially in the near and mid infrared spectral regions, where it is mostly referred to as Fourier Transform Infra-Red (shortened to FTIR) spectroscopy. “

Lines 38-42: ATMOS should be mentioned here; the first high-resolution FTIR spectrometer to fly in space. Farmer, Crofton B. (1987), High resolution infrared spectroscopy of the sun and the earth's atmosphere from space. Mikrochimica Acta, 93. 189-214 doi:10.1007/bf01201690

Lines 17 & 19: The authors use the word “connect” to express the relationship between the interferogram domain and the spectral domain. For example, it is used twice in the first four lines of the abstract: “...for concluding which spectral distribution **connects** with the measured interferogram. We present implementation of an improved scheme for phase determination in the operational Collaborative Carbon Column Observing Network (COCCON) processor. We introduce a robust unwrapping scheme for retrieving a **connected** phase spectrum...”. To me, “connected” is too vague term. I’m not sure what it is supposed to convey. So, I suggest replacing the first “connects” and deleting the second as follows:

“...for concluding which spectral distribution **most likely gave rise to** the measured interferogram. We present implementation of an improved scheme for phase determination in the operational Collaborative Carbon Column Observing Network (COCCON) processor. We introduce a robust unwrapping scheme for retrieving a phase spectrum....”

Line 21: “suited” → “suitable”?

Line 31: Here you use the term Fourier Transform Spectrometry, which I believe is correct. In other places you speak of absorption “spectroscopy”, e.g., lines 62-70 contain 4 instances. Are you using the words “spectroscopy” and “spectrometry” interchangeably, or are you making a subtle distinction? If the latter, please explain in the paper. IMO all instances should be “spectrometry” since “spectroscopy” is the study of the interaction of electromagnetic radiation with matter, which is not what TCCON or COCCON do.

Line 73: “maximum optical path difference (MPD) is“ Why doesn’t “optical” participate in the acronym (MOPD)?

Lines 75-76: “A proper description of the instrumental line shape (ILS) is further complicated due to the presence of practical imperfections of the interferometer. “
Need to give an example or two of these “practical imperfections”, or add “as will be shown later”.
Otherwise, the reader is left hanging.

Line 90: You don’t mention the compensator here. Surely, the mismatch in thickness and/or refractive index between the beamsplitter and compensator is a major cause of phase error.

Line 97: The term $S(v)$ multiplies the integral in equation (1), but here in eqtn (2) it is equal to the integral. Is there a missing “=” in eqtn. (1)?

Line 97: Earlier (line 74) it was mentioned that the interferogram is multiplied by a boxcar function. Why is this not shown in eqtn (2)?

Line 107: “The assumption of uncorrelated white noise typically is adequate“. Adequate for what purpose?

Line 111: “The assumption of a spectrally smooth phase allows to separate at each spectral position the complex spectrum into two orthogonal components”
“allows to separate” is a construction that is not used in English speaking world. I suggest re-writing as: “The assumption of a spectrally smooth phase allows separation of the complex spectrum into two orthogonal components”

Line 112: Please clarify what you mean by “direction”.

Line 131: “Instead, the ZPD position shifted near one end of the mechanical scan range”
Re-write as “Instead, the ZPD position is shifted to be near one end of the mechanical scan range”

Line 132: I think that “equation (2)” should be “equation (3)”.

Lines 151 to 188: This section interrupts the flow of the scientific discussion, by providing a lot of mostly irrelevant information about the various Bruker spectrometers. For example, the fact that they use the “Rock-Solid” design is mentioned twice here, as is the fact that “more than 100 units are sold”. This

section should be considerably shortened, or moved to an appendix. Perhaps cite the Bruker website/brochure for readers who want this type of information.

Lines 191-195: “IZO is managed by the Izaña Atmospheric Research Centre (IARC, <https://izana.aemet.es/>, last access: 5 August 2024), which belongs to the State Meteorological Agency of Spain (AEMet). Within the IZO’s atmospheric research activities, the FTIR programme started in 1999 in the framework of a collaboration between AEMET and KIT [Schneider et al., 2005], contributing to NDACC and TCCON networks since 1999 and 2007, respectively.”

I don’t find this mostly historical information scientifically relevant. Which organizations manage and fund the IZO site, and how long they have done so, are not relevant to phase correction. Most of this should be moved to the Acknowledgements. The website <https://izana.aemet.es> contains nothing of relevance to phase correction. Also, the paragraph doesn’t mention COCCON, which I thought was the main driver of the new phase correction method.

Line 170: “1mm” → “1 mm”. In most places a space is left between the value and the unit, but here not.

Line 198: “Schneider etThis al. “ → “Schneider et al.”

Lines 202-215: “Because the phase spectrum across such a region is strongly impacted by the overlapping contributions to the phase emerging from either side of the opaque region, the outcome for the phase at a certain spectral position in the region with reduced transmission will depend on the user-selected resolution for the phase calculation and the chosen apodization function.”

I don’t dispute this statement – this is what you found. But it doesn’t explain why the phase correction operator is so sensitive to the user-selected resolution or apodization. The exact phase value will of course have some dependence on the interferogram points selected (i.e. the phase resolution) and their relative weighting (i.e., apodization). But why does this have a large effect on the phase?

Also, It seems contradictory that points far from ZPD contain some information about the phase, that you wish to retain, but you subsequently fit a low-order polynomial through the phase, which is smoother, and therefore contains no high-resolution frequencies coming from igran points far from ZPD.

Lines 227-229: “This proposed method can fail if the phase difference calculated in step 5 is greater than $\pm\pi$. We did not encounter this situation, but it may occur if the phase slope is very steep and can possibly be avoided by appropriate repositioning of the ZPD point when calculating the Fourier Transform. This is of concern because when automatically processing thousands of interferograms, how would we know when the ZPD point needs to be repositioned?”

Table 1: “logical array indicating availability of valid phase value “ → “logical array indicating validity of phase value”

Table 1: Why isn’t $s(v_i)$ allocated in step 0?

Table 1: Perhaps give names to the float array containing phase and the logical array containing validity e.g. Psi and LVALID. This would avoid repeating “logical array value of current position“ later in the table (twice).

Table 1: “Use the value of the cross product between the normalized complex pointers”
What are “normalized complex pointers”? There is no mention of “pointers” anywhere else in the paper.

Table 1: At which step is index j updated? Somewhere it is set to i , before i is incremented.

The equation $\Delta\phi_{(j \rightarrow i)} = \text{asin}\{\}$ in Table 2 finds the phase difference between the complex vectors Sv_i and Sv_j by using their cross product. It is not obvious why this is the case. To me, it would be simpler to directly subtract the phases at v_i and v_j as follows:

Let $Sv_i=[a+ib]$, $Sv_j=[c+id]$, where $i=\text{Sqrt}(-1)$. The phase of Sv_i is $\text{atan}[b/a]$ and that of Sv_j is $\text{atan}[d/c]$.

$$\Delta\phi_{(j \rightarrow i)} = \phi_i - \phi_j = \text{atan}[b/a] - \text{atan}[d/c] = \text{atan}[(ad-bc)/(ac+bd)]$$

To me this approach seems more intuitive than using cross-products. So please explain the advantage using a vector product, rather than simply subtracting the two phases.

Table 1: Where does the “phase unwrapping” occur? This is mentioned earlier in the paper including the abstract. But then nothing more.

Line 226: Here Table 1 is mentioned, but there is no description in the main body of text. So the table itself and its caption need to be more self-explanatory.

Line 234: “The second step...”. At first, I thought that this referred to Table 1 (Step #). But that doesn’t make sense. So perhaps change this sentence to “After completing the raw phase vector over the full bandwidth, as described in Table 1, we next fit the parameters of the phase model to the raw phase values.”

Line 247: Need to clarify whether *Pmodel* is the retrieved model parameters (e.g., polynomial coeffs) or the reconstructed phase values. Line 247 states “*Pmodel* is the set of model parameters”. But line 250 states “after receiving the set of model parameters, *Pmodel* can be calculated at all spectral positions”, which suggests that *Pmodel* is the reconstructed phase values themselves.

Line 256: “phase calculation uses a resolution of about 10 cm^{-1} , which is supported by all spectrometers we included in the study (sufficient number of points on the short side of the interferogram).” It would be helpful to some readers to also express this as interferogram points. Assuming the usual two samples per reference laser wavelength, I think that 10 cm^{-1} corresponds to a MOPD of $0.9/10=0.09 \text{ cm}$ which is $0.0/0.3154\text{E}-04=2844$ interferogram points on each side of ZPD. If correct, perhaps state this number.

Figure 1: Why does the right-hand panel have a slightly narrower wavenumber range than the left-hand panel, or figs. 2, 3, 4.

Line 269: “model (analytical, ana)”. What is “ana”? I puzzled over this for a while before deciding that you are defining a new abbreviation. But why not simply label the y-axes of the figs “analytic - raw” – there’s plenty of room. The “ana” abbreviation isn’t used anywhere else.

Line 269: Is the “fitted model (red)” the same thing as “model (analytical, ana)”? If so, use the same terminology. If they are different, explain the distinction.

Line 283: “The curvature of the phase is somewhat stronger than in case of the IRCube.” → “The curvature of the phase is somewhat stronger than in **the** case of the IRCube.”

Line 308: “Figure 5 shows the effect of using either the Mertz or the analytical phase “ → “Figure 5 shows the effect of using either the **classical** Mertz or the analytical phase...”

Line 316: “This reminds of the fact that...” → “This is a reminder of the fact that”

Line 320: “...phase reconstruction is of higher importance for single-sided interferograms (all the spectrometers investigated here apart from the EM27/SUN) than for the EM27/SUN, which essentially is insensitive to phase errors in reasonable limits” This is a bit clumsy. I suggest re-writing as: “...phase

reconstruction is much easier and accurate for double-sided interferograms (i.e., the EM27/SUN) than for single-sided interferograms (the other spectrometers discussed here)”

Line 323-326: Split into two sentences.

Line 326: Needs a reference for why atmospheric xCO₂ measurements need an accuracy of 0.05 ppm.

Line 328: Is $2 \cdot 10^{-5}$ a fractional change? So this is a $425 \text{ ppm} \cdot 2 \cdot 10^{-5} = 0.0085$ ppm change in xCO₂. This is very small. So for the EM-27 or the IR cube, the classical Mertz phase correction is perfectly adequate.

Line 333: How much difference between the two phase correction methods for the Vertex and IFS125? These instruments seem to have been dropped from the discussion.