

FRM4GHG 2.0

Fiducial Reference Measurements for Greenhouse Gases



Technical Note on PROFFAST update in support of
different types of low-resolution spectrometers

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Lead author(s):	Frank Hase (KIT)
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1 DOCUMENT CHANGE RECORD

Issue	Date	Item	Comment
V1.0	2024-08-15	-	Initial version

2 ACCESS LIST

This document is a deliverable “D2.1.1: PROFFAST updates” – created for the project FRM4GHG 2.0 and will be submitted to ESA. The document can be downloaded from the project webpage <http://frm4ghg.aeronomie.be>.

3 PURPOSE

The document describes extensions incorporated into the COCCON processing chain in order to support the data analysis for all low-resolution Fourier transform infrared spectrometers operated within FRM4GHG 2.0. Apart from the EM27/SUN, the other spectrometers deliver single-sided interferograms, so the COCCON pre-processor needs to handle single-sided interferograms. The calculation of the phase spectrum becomes a critical task in this context, and we show here how this problem has been solved.

4 DOCUMENT STRUCTURE

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5 PROFFAST SUPPORT FOR DIFFERENT TYPES OF FTIR SPECTROMETERS

Support for different spectrometers required some technical extensions in the PROFFAST code, which have been implemented: support of different spectral resolutions, support of variable amount of self-apodisation due to different instrumental field-of-views, and support of different file structure in the measured data (according to spectral coverage of primary and secondary detector branch, if any). Beyond such technical extensions is the handling of single-sided interferograms, which are more sensitive to the presence of phase errors than the double-sided interferograms as provided by the EM27/SUN FTS. We therefore have implemented a novel phase reconstruction scheme, which we discuss in more depth in this report. The successful implementation of all the required additional functionalities in PROFFAST has been verified by

processing test data of the IRcube, and the Vertex70 and Invenio provided by the FRM4GHG project partners.

5.1 A novel approach for phase correction for FTIR solar absorption spectrometry

Due to the presence of optical asymmetries and electronic delays between infrared and reference laser processing circuits, the interferograms delivered by an FTIR spectrometer are asymmetric. The degree of asymmetry and the evolution of asymmetry as function of wavenumber is described by the phase spectrum. Traditionally, the expectation that the phase is spectrally smooth is exploited by deriving the phase from a narrow double-sided section of the interferogram windowing the centerburst of the interferogram. The drawback of this Mertz phase correction scheme is that the resulting smoothing is not well-defined (depends on selected phase resolution, distribution of spectral flux, and choice of numerical apodisation). Learner et al, 1995, proposed an alternative scheme for emission spectra, which we apply here for solar absorption spectroscopy. It consists of two steps: (1) a robust phase unwrapping scheme and (2) fit of an analytical phase model to the unwrapped phase.

Figure 1 shows the result of the new scheme for the EM27/SUN FTS.

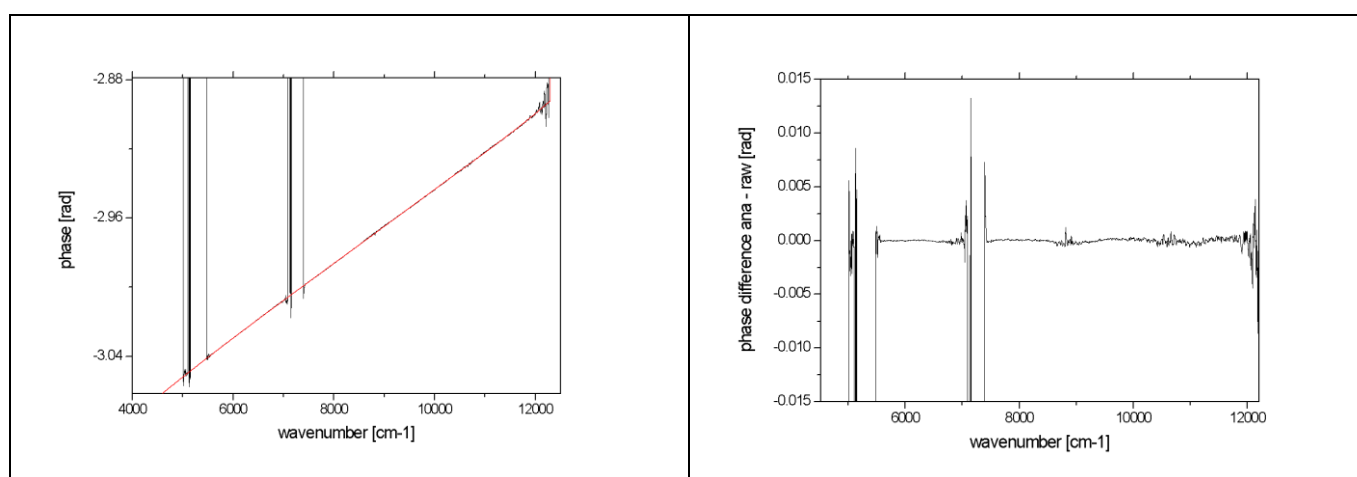


Figure 1: Fit results for the EM27/SUN phase (adopted from Hase et al., 2024). Left panel: unwrapped and fitted analytical phase; right panel: difference between unwrapped and analytical phase.

5.2 IRcube phase spectrum

The phase results for the IRcube are similar to the EM27/SUN results, due to a similar type of interferometer (and processing electronics) being used in this spectrometer.

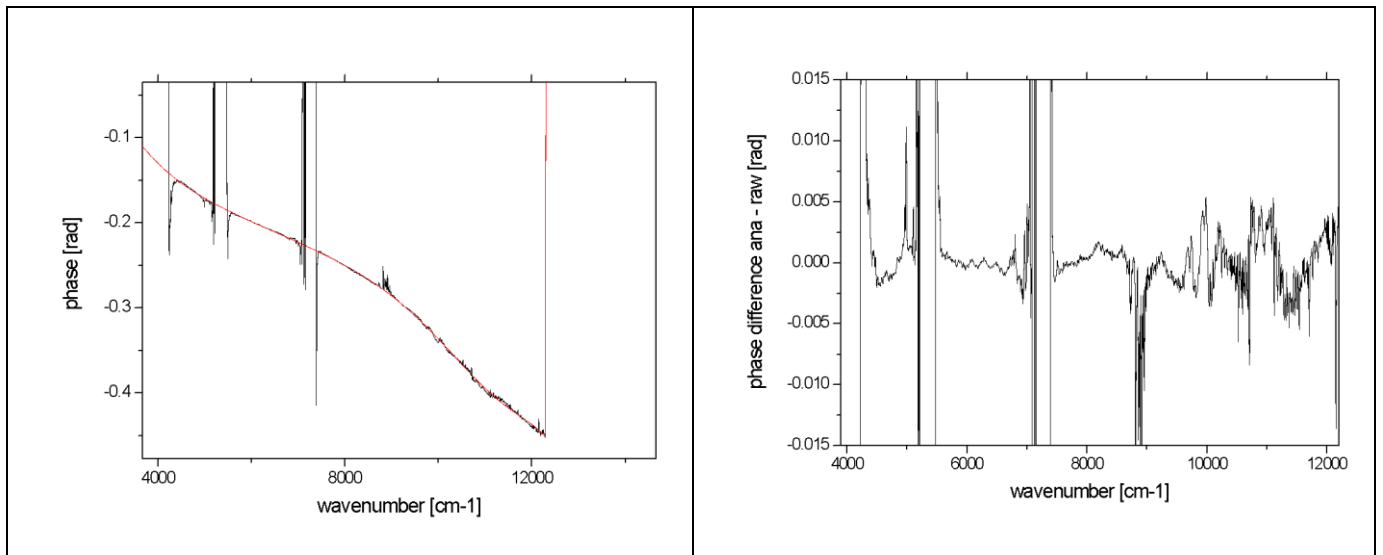


Figure 2: Fit results for the IRCube phase (adopted from Hase et al., 2024). Left panel: unwrapped and fitted analytical phase; right panel: difference between unwrapped and analytical phase.

The phase spectrum of the IRCube is less straight than that of the EM27/SUN, which suggests that the compensated beamsplitter design (the same plate acts as beamsplitter substrate and as compensation plate in subsequent passes) realized in the EM27/SUN is not fully incorporated in the IRCube.

5.3 Vertex 70 / Invenio phase spectrum

The Vertex 70 and Invenio phase spectra have somewhat stronger deviations from a straight line as the IRCube. Surprisingly, the phase shows an undulation of about 500 cm⁻¹ repeating cycle. The instrumental origin of this feature (shared by the Vertex 70 and Invenio) is unknown. Confronted with our findings, also the manufacturer Bruker has no explanation for this unexpected peculiarity from the design viewpoint.

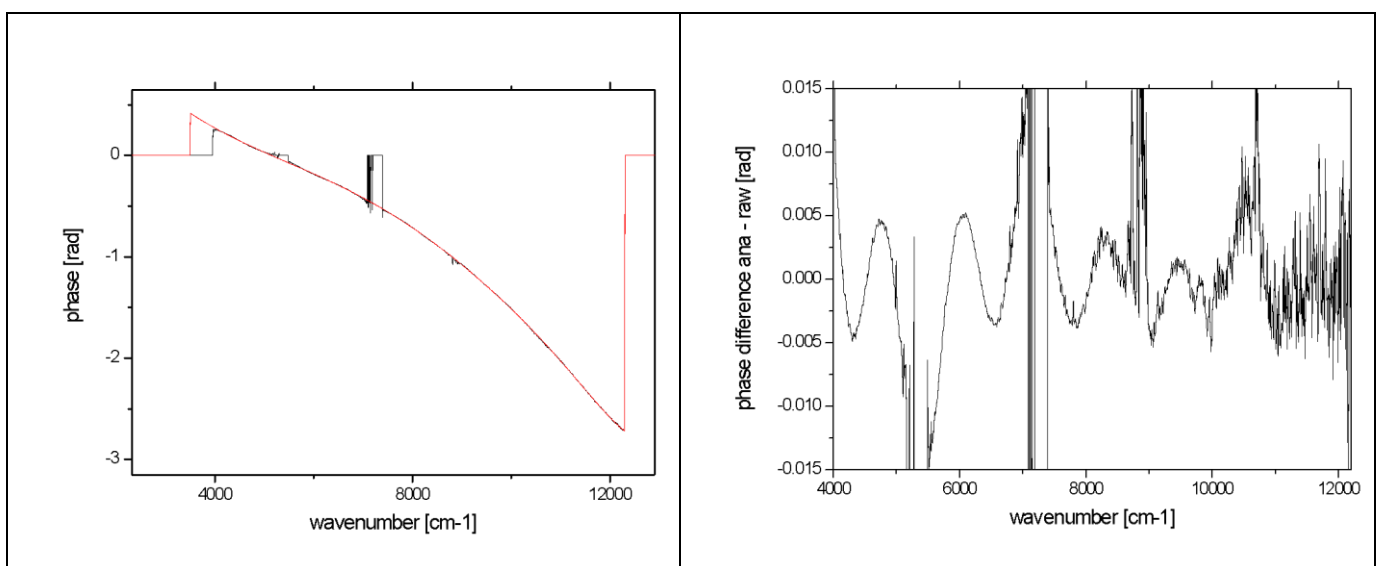


Figure 3: Fit results for the Vertex70 phase (adopted from Hase et al., 2024). Left panel: unwrapped and fitted analytical phase; right panel: difference between unwrapped and analytical phase.

5.4 Conclusions and perspectives

The new scheme implemented in PREPROCESS allows to process single-sided interferograms, as recorded with the IRCube, and the Vertex70, and its successor Invenio. The option of an analytical phase in addition to the standard approach allows a critical review of spectral structures in the phase spectrum. The new implementation as introduced here is described in a journal article submitted to AMT (AMT-2024-140, submitted on 2024-Aug-09).

6 APPLICABLE DOCUMENTS

Statement of Work: Fiducial Reference Measurements for Ground-Based IR Greenhouse Gas Observations (FRM4GHG 2.0)
Prepared by: EOP-GMQ, Reference: ESA-EOPG-EOPGMQ-SOW-21

7 REFERENCE DOCUMENTS

Frank Hase, Paolo Castracane, Angelika Dehn, Omaira Elena García, David W. T. Griffith, Lukas Heizmann, Nicholas B. Jones, Tomi Karppinen, Rigel Kivi, Martine de Mazière, Justus Notholt, and Mahesh Kumar Sha: "Implementation and application of an improved phase spectrum determination scheme for Fourier Transform Spectrometry", submitted to AMT, 2024.

Richard C. M. Learner, Anne P. Thorne, Ian Wynne-Jones, James W. Brault, and Mark C. Abrams: Phase correction of emission line Fourier transform spectra, *J. Opt. Soc. Am. A* 12, 2165-2171, 1995.

Sha, M. K., De Mazière, M., Notholt, J., Blumenstock, T., Chen, H., Dehn, A., Griffith, D. W. T., Hase, F., Heikkinen, P., Hermans, C., Hoffmann, A., Huebner, M., Jones, N., Kivi, R., Langerock, B., Petri, C., Scolas, F., Tu, Q., and Weidmann, D.: Intercomparison of low- and high-resolution infrared spectrometers for ground-based solar remote sensing measurements of total column concentrations of CO₂, CH₄, and CO, *Atmos. Meas. Tech.*, 13, 4791–4839, <https://doi.org/10.5194/amt-13-4791-2020>, 2020.