

General notes on the COCCON software package including the PREPROCESS and PROFAST tools

Contents of distribution

This software package contains executable files for Windows and Linux systems. The pre-processing tool is located in the "preprocess" folder ("preprocess4.exe" for Windows and "preprocess4" for Linux). The retrieval tools are in the main folder named "prf96-EM27-fast" ("pcxs10.exe" and "invers10.exe" for Windows, "pcxs10" and "invers10" for Linux). The Windows executable files were generated with an Intel compiler (Intel Parallel Studio XE 2019 Professional) that requires a 64-bit architecture. The Linux files were compiled under an Ubuntu OS (i.e. Ubuntu 16.04 LTS, 64-bit system) using the GNU Fortran compiler 5.4.0.

The source codes for both the Windows and the Linux version are included in this software distribution. They are placed into the folder for the auxiliary files (i.e. "auxil"). These source codes can also be compiled by the end user in case of any problems with the precompiled executable files. Several Fortran compilers for Windows OS are commercially available (e.g. the Intel or the Lahey compiler). The free GNU Fortran compiler is available for both Windows and Linux platforms. Any compiler supporting the Fortran 2003 standard should be suitable for generating executables from the provided source codes.

Functionality and procedures

The result of the measurement is an interferogram in OPUS format. The PREPROCESS program is used to generate spectra from these raw measurements, performing a DC correction, an FFT including phase correction, and quality filtering / flagging. From a measurement passing the QC, a spectrum in *.bin format is generated by PREPROCESS.

The quantitative trace gas analysis is performed in two steps for each day. Firstly, the pcxs10 code is used for tabulating the x-sections of all relevant gases as function of a pressure-temperature profile and the assumed trace gas profiles (for compatibility with TCCON, we recommend to use the daily *.map file generated by TCCON for your site). The retrievals for each individual spectrum are performed using invers10, the tabulated ground pressure and optionally the PBL temperature are used in this step (to reflect the intraday variability of the ground pressure, PBL temperature might be assumed constant if no further information is available). Results of the quantitative trace gas analysis are the XVMR results, airmass independent and airmass dependent corrections are taken into account in invers10, so no separated post-processing step is required.

How to run the sample files included

The procedure for the Linux version is as follows: First, check whether the settings for the provided executable files are correct. Therefore, open a command line and change to the corresponding folder of the executable files (i.e. "prf96-EM27-fast"). Then, type the command "ls -l" to list the directory contents using a long listing format. Alternatively, type "ls -l pcxs10", "ls -l invers10" or "ls -l preprocess/preprocess4" to see the details of the executable files only. The beginning of each line should ideally be: "-rwxrwxr-x". If this is not the case and the beginning of the line differs somehow (e.g. "-rw-r--r--"), the file mode has to be changed. Type "chmod +x preprocess/preprocess4", "chmod +x pcxs10" and "chmod +x invers10", respectively, to change the file mode bits. Execute the files by typing "./preprocess4" (in the "preprocess" folder), "./pcxs10 pcxs10.inp" and "./invers10 invers10.inp" (in the main folder). However, one should bear in mind to edit the input files (i.e.

"preprocess/preprocess.inp", "inp_fast/pcxs10.inp" and "inp_fast/invers10.inp"). The input files contain, among other things, the relative and absolute paths which have to be adjusted. Please note, that backslashes are used for the path specifications on a Windows OS and slashes for those on a Linux OS. On a Windows system, the executables "preprocess4.exe", "pcxs10.exe", and "invers10.exe" have to be executed instead.

Recompiling the Linux executables

If the executable files still are not working properly, a compilation of the source code by the user is advised. Here, only the instructions for a Linux system are presented shortly. First, change to the directory of the source code that is stored in the folder for the auxiliary files for both operating systems, separately (i.e. "auxil"). Then, type the corresponding command lines within each folder:

```
"gfortran -O2 -o preprocess4 glob_prepro4.f90 globOPUSparms.f90 preprocess4.f90",  
"gfortran -O2 -o pcxs10 globvar10.f90 globlin10.f90 globlev10.f90 pcxs10.f90", and  
"gfortran -O2 -o invers10 globinv10.f90 inver10.f90".
```

The command "gfortran" has to be replaced by the installed Fortran version (e.g. "gfortran-4.6" or "gfortran-5"). To find out, which Fortran version is installed on your system, simply type "gfortran" and use the tabulator key twice. Assuming, that the compilation was performed without an error message, the file modes should be checked again and corrected if necessary (see explanation above). Next, copy the resulting "preprocess4" file to the "preprocess" folder and overwrite the existing file. The same applies to the files "pcxs10" and "invers10", which have to be replaced in the main folder. Finally, the instructions for the execution of the preprocessing and retrieval files, that have been summarized previously, can be repeated.

PROFFAST Release Notes

January 17, 2019 Beta Version of the Software Distribution

Updated March 26, 2019 Bug Fixes (reported by Melissa Kouassi, LSCE)

The length of the string containing the retrieval results for a certain day was not set correctly. The output file of the inverse calculation containing an additional character at the end of each line could be misinterpreted. Therefore, the string length was corrected and as a result of this the additional character removed.

Updated July 23, 2019 Bug Fix (reported and resolved by Nicholas Jones, UoW)

The Julian date is derived from time and date provided in the OPUS file. An optional time offset defined in the input file of the preprocessing tool can be applied, if time and date stored in the OPUS file refer to the local time zone instead of Greenwich (UTC). If this option was used, the evaluation of the readjusted time was incorrect (using seconds instead of hours as required) and resulted in an incorrect date.

Updated August 9, 2019 Software Extension

The software package is now extended by an additional beta version supporting low-resolution double-sided measurements recorded with IFS125HR spectrometers (low-res observations performed at several TCCON sites) which is located in the directory "preprocess-ttcon". Double sided interferograms recorded with the IFS 125HR spectrometer can now be handled if the spectrometer is operated in an EM27/SUN compatible mode applying 0.5 cm⁻¹ resolution (which corresponds to a

maximum optical path difference of 1.8 cm). An optional input file named "tcon.inp" was created to ensure the compatibility of the primary preprocessing input files "preprocess4.inp" used for the EM27/SUN measurements. This optional secondary input file contains the information whether the interferograms of the OPUS files are covering the extended InGaAs spectral range (which is the standard TCCON setup) or whether the CO band is observed with a separate detector (TCCON setup Karlsruhe). Apart from this extension, the extended tool supporting low-res TCCON measurements is identical to the current consolidated version of preprocessing tool (and will replace the current standard distribution after a testing phase).

Updated November 11, 2019 Software Extension

This code version provides partial column sensitivities (daily ASCII tables, sensitivity vectors for each species tabulated as fct of SZA). The calculation is incorporated into the pcxs10.exe, the sensitivities are generated together with the daily lookup table containing the molecular x-sections when pcxs10.exe is called. The results can be found in out_fast in the "XXXYMMDD-colsens.dat" file.

IMPORTANT, PLEASE NOTE:

Because the transmission used for the calculation of the column sensitivities is calculated on the fly, the sequence of absorbers in the state vector has been changed. The strong absorber CH₄ now precedes N₂O and CO. Apart from the changed sequence and provision of column sensitivities, no changes were made wrt the previous distribution, so apart from the ordering the trace gas results remain unchanged.

IMPORTANT, PLEASE NOTE: (Homepage)

The species order in the state vector has been changed. See new input files.

Updated February 28, 2020 Bug Fix

New SW bug discovered and solved in the add-on functionality of the PREPROCESS tool in support of TCCON (second channel output was suppressed in case of low-res evaluations of IFS125HR spectra).

Updated June 26, 2020 Bug Fixes, and Python Tools

Inconsistent initialization of auxiliary variables fixed. Values as set in parameter module are now consistently used (no separate initialization in subroutines). Flexibility increased (work towards supporting higher resolution spectrometers, e.g. Vertex22) - for this purpose, the input file has been slightly extended. Inconvenient code behavior of PROFFAST inversion (stops and prompts error occurrence to operator, typical error states: either ATA matrix near singularity or spectral shift too big). For improving the code behavior, a Levenberg-Marquardt (LM) scheme has been implemented. If the ATA matrix is found to be nearly singular, the LM damping procedure is entered. If the spectral shift exceeds the allowed bounds, its value is limited to the maximum allowed range.

The tool collection consists of several Python scripts guiding the user step-by-step through the evaluation process of the EM27/SUN measurements. A detailed description of the tool collection is enclosed in the PROFFAST software compilation.

Updated July 15, 2020 Bug Fix, and Output Extension

A LM stabilization scheme was included (which activates in convergence problems are detected). The solar azimuth angle is now provided in the output file.

Updated August 10, 2020 Bug Fix, and Output Extension

An array allocation order has been corrected (array fullmesspec1: field element zero was used, while array started at 1). The observer coordinates are now provided in the output file.

Updated February 5, 2021 Software Extension, and Python Tools

Enable time shift (optional input file) for aligning spectra naming time zone with time zone used in intraday pressure file. Introduction of a new input file (i.e. "General-Input-File.inp") used by the given Python scripts for processing large data sets. The input file contains all paths and directories that were previously stored separately within the scripts. Additional Python scripts are provided for creating/generating GEOMS compliant HDF files (both HDF4 and HDF5 files).