Update COCCON processing

Collaborative Carbon Column Observing Network

COCCON-OPERA

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https://frm4ghg.aeronomie.be/

COCCON processing

The COCCON data processing chain has three steps:

(1) PREPROCESS: Generates spectra from raw interferograms

(2) PCXS: Generates daily lookup tables informing about x-sections of gases

(3) INVERS: Trace gas retrievals for all spectra measured during a day

This talk presents two recent code updates in the operational ver 2.4:

(a) PREPROCESS – support of variable observer coordinate

(b) PCXS – faster generation of xsc-lookup table

And two further code updates in the current internal beta version:

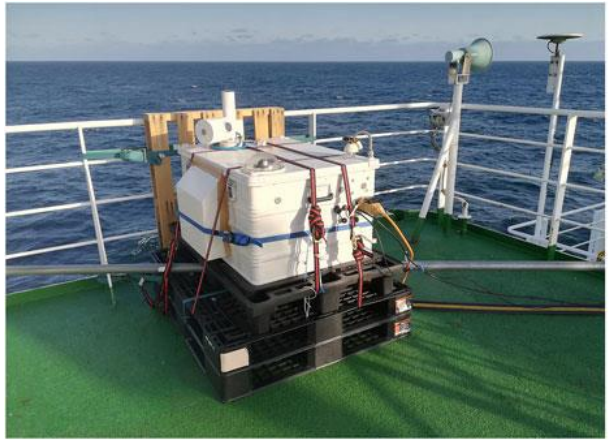
(c) nonlinearity correction for the EM27/SUN

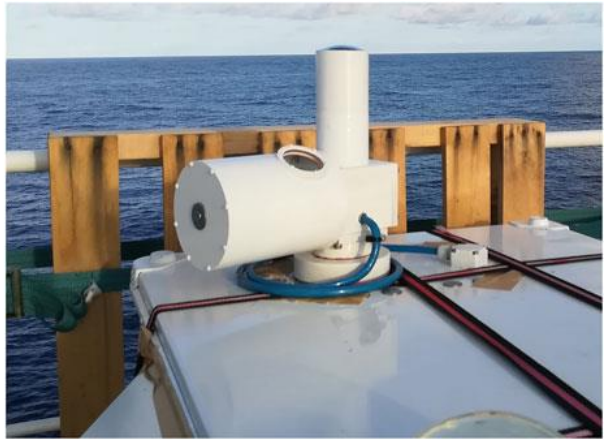
(d) residual solar Doppler scale diagnostics

COCCON processing: PREPROCESS

Background: meanwhile, UHD (A. Butz, R. Kleinschek, …) and NIES (A. Müller, M. Frey, …) are taking regular ship measurements on a cargo vessel travelling along the Japanese coast line. The investigators would kindly provide their data to COCCON!

Side-by-side meas at KIT





EM27/SUN onboard RV Mirai

COCCON processing: PREPROCESS

Envisaged procedure:

(1) PREPROCESS needs to accept variable observer coordinates

(2) A daily map file for the ship‘s noon coordinate is requested

(3) The pressure data measured on board is used by INVERS (no change here)

TBD:

✓ Extension of PREPROCESS code

- Extensions on the wrapper:

  generate PREPROCESS input (use ship track)

  request map file for noon coordinate

Note: If use of a single noon map file would turn out to be a too coarse approach, the measurement day could be splitted in a few subperiods.

COCCON processing: PREPROCESS

Relevant sections from standard preprocess.inp:

T/F: fixed or variable observer coordinates
specify site name
specify time offset of OPUS time versus UT (hours+decimals)
if fixed observer coordinates: specify fixed observer coords (lat_deg,long_deg (East pos),alt_km)

$
.true.
sodankyla
0.0
67.366 26.63 0.181

…

list of raw measurements (path and filename, end marker ***)
$
D:\prf96-EM27-fast\preprocess\sod#6\170608\170608SN.0
D:\prf96-EM27-fast\preprocess\sod#6\170608\170608SN.1
D:\prf96-EM27-fast\preprocess\sod#6\170608\170608SN.10
D:\prf96-EM27-fast\preprocess\sod#6\170608\170608SN.100
***

COCCON processing: PREPROCESS

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D:\prf96-EM27-fast\preprocess\sod#6\170608\170608SN.0,67.366,26.63,0.181
D:\prf96-EM27-fast\preprocess\sod#6\170608\170608SN.1,67.466,26.53,0.181
D:\prf96-EM27-fast\preprocess\sod#6\170608\170608SN.10,67.566,26.43,0.181
D:\prf96-EM27-fast\preprocess\sod#6\170608\170608SN.100,67.666,26.33,0.181
***

COCCON processing: PCXS

PREPROCESS and INVERS are pretty efficient, the currently distributed version of PCXS requires ~ 7 min (single core, Intel i7-3770 CPU @ 3.40GHz) for generating the required lookup table.

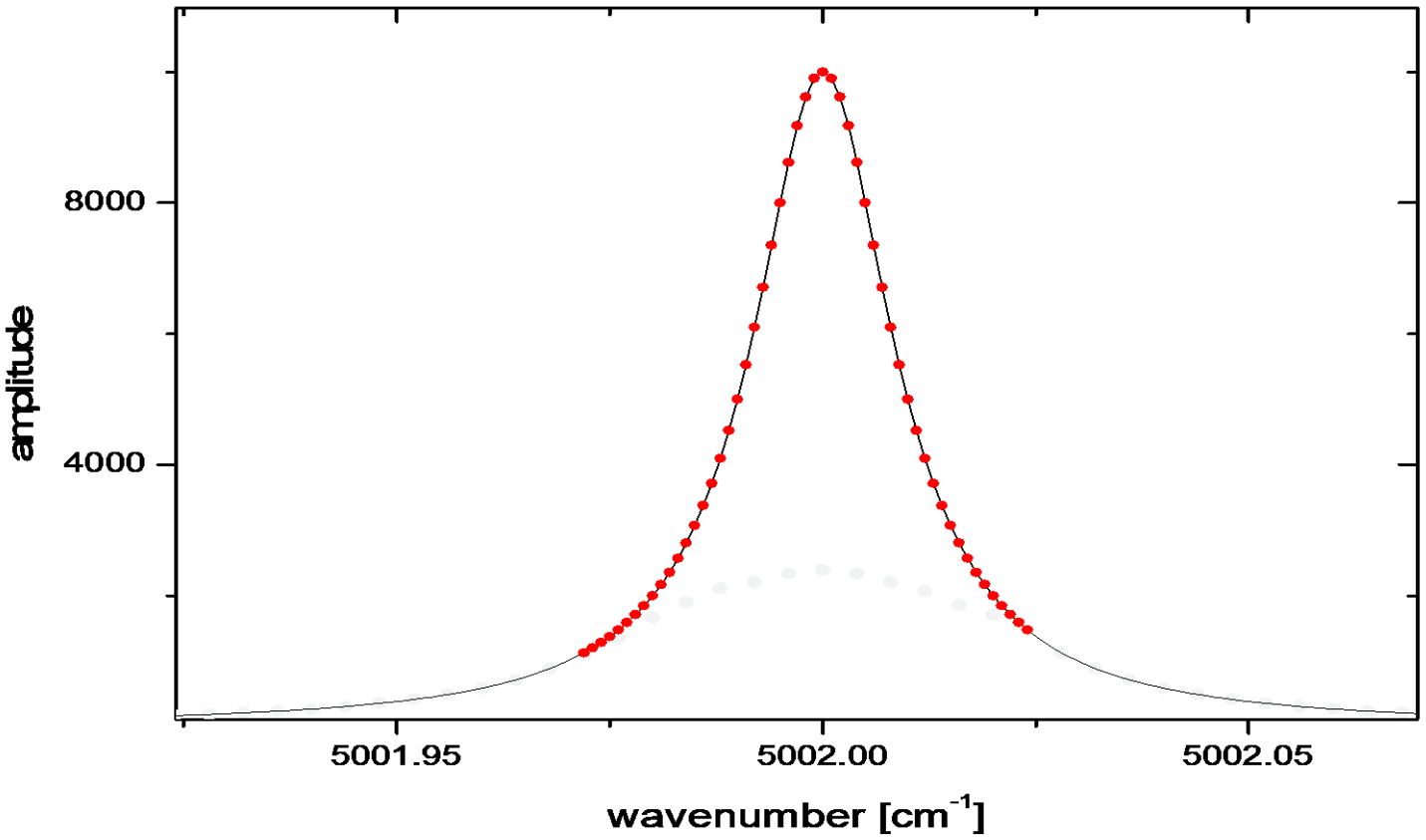
For (re)processing of a large number of measurement days, the computational effort for PCXS becomes noticeable, a reduction of computational effort is desirable.

Current scheme:
Each line contribution (Voigt + extensions (LM, SDV)) is added on each spectral grid point of a fine global spectral grid ($\pm 25\ cm^{-1}$).

New scheme:
Each line contribution is split in two parts. The first part contains the narrow section around the line center peak (sampled on the fine global spectral grid. The remaining second low-res part is sampled on a coarser spectral grid ($\Delta\nu_{coarse} = 4\Delta\nu_{fine}$). After collecting all line contributions, the coarse grid contribution is interpolated and added on the fine grid.

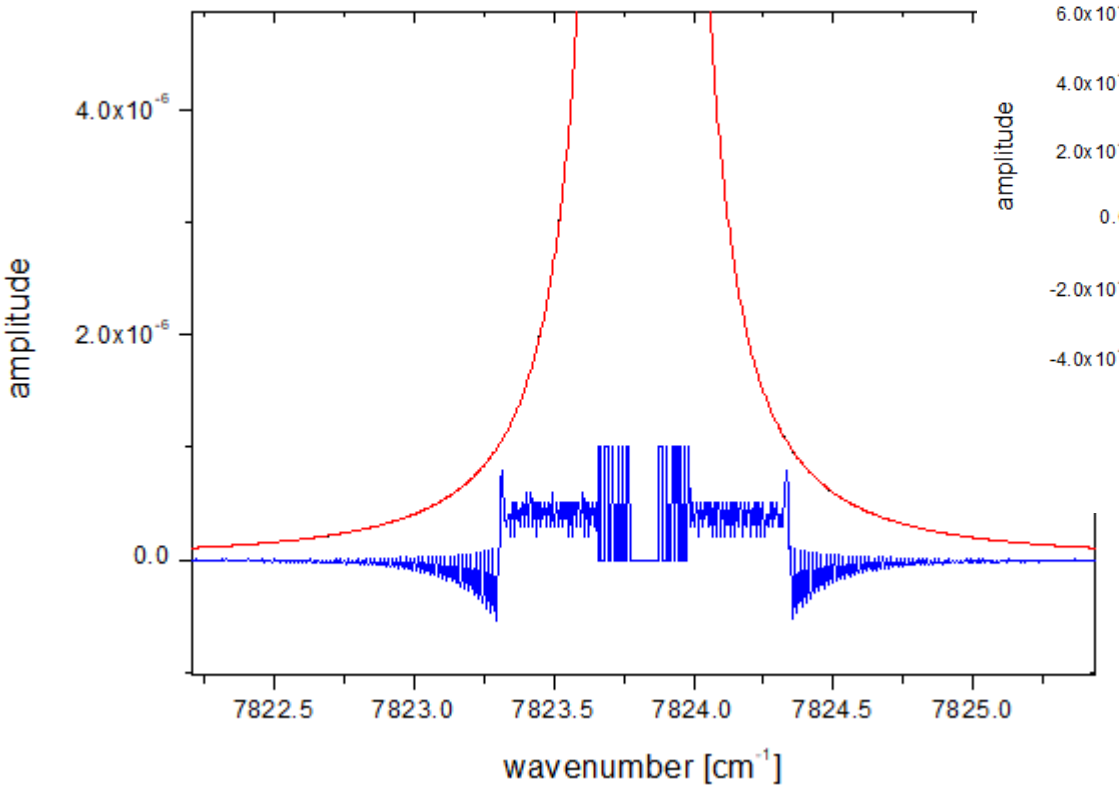
COCCON processing: PCXS

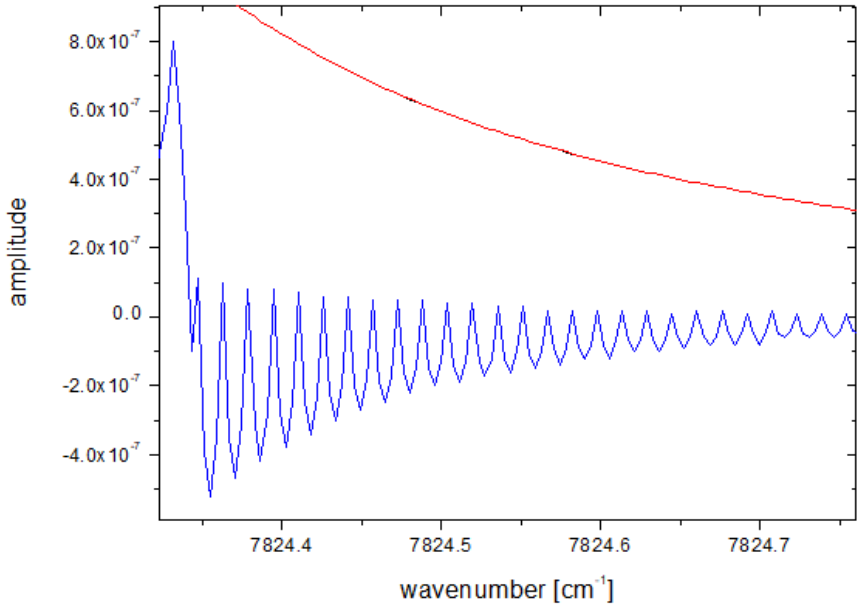
Graphical outline of the procedure (a smooth polynomial replacement for completion of the coarse grid contribution is used. This needs to be subtracted from the fine grid contribution):



COCCON processing: PCXS

Effects on modelled line shapes (difference x 1000)





COCCON processing: PCXS

Effects on XGAS:

XH2O ~7e-5
XCO2 ~8e-5
XCH4 ~1e-5
XCO ~2e-5

Speed gain for creating one table: 7 min -> 1 min 40 s

We plan to include these updates in the next PROFFAST release (2.4):

- New PREPROCESS code
- New PCXS code

Final adjustment of gas-specific tying of COCCON XGAS scale to TCCON is under construction (AICFs, ADCFs, XH2O dependence): BH + JV

COCCON processing: Nonlinearity correction

- Nonlinearity correction scheme implemented (for operational use)

  Two-step procedure:

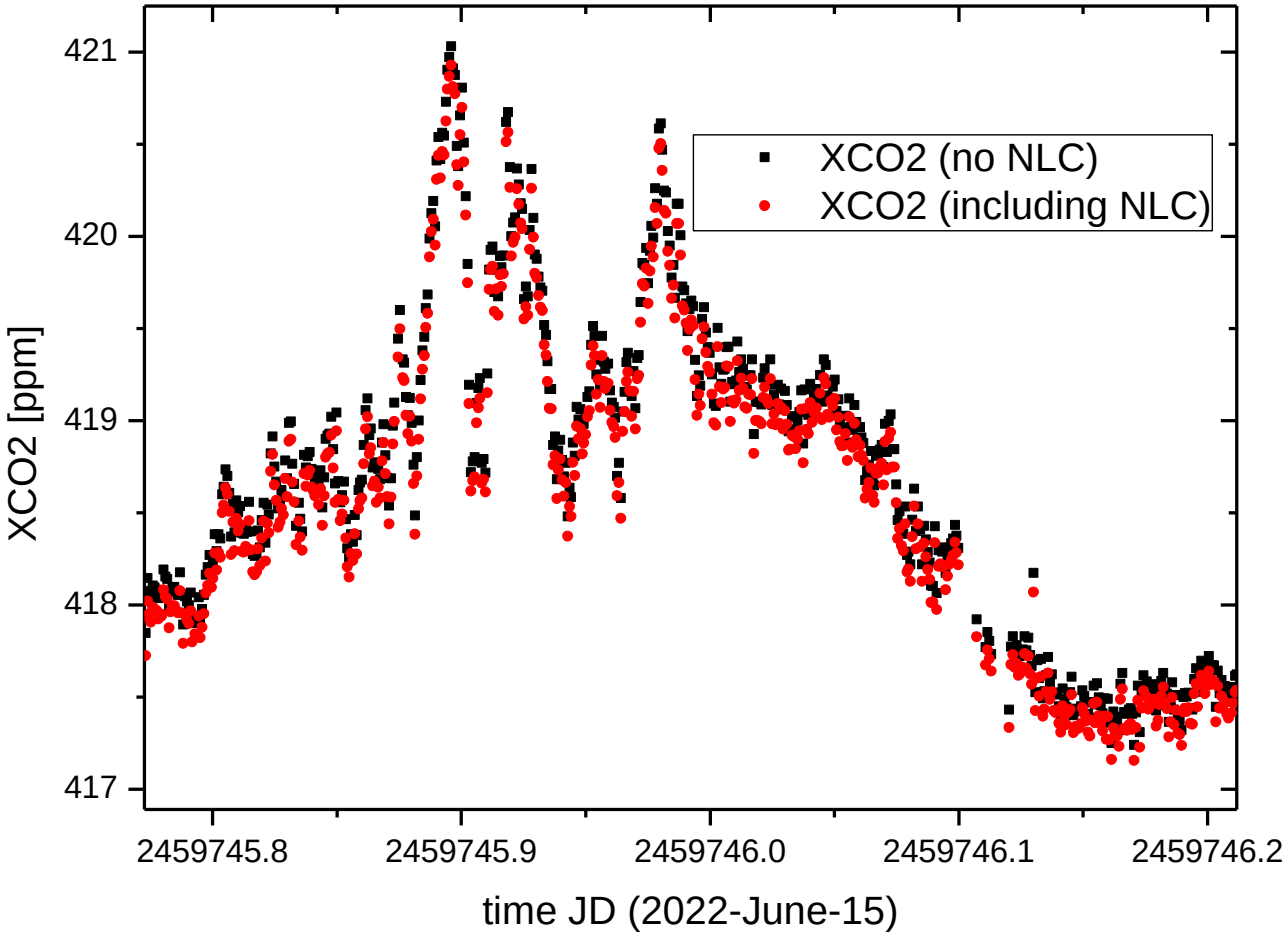
  Step (1):

  - Perform fit of characteristic curve (using dedicated PREPROCESS option: based on a set (~12) of selected measurements), result: set of parameters
  - This task needs to be done for all pre / gain configurations used on spectrometer SNXXX

  Step (2):

  - Add table of parameters for all required pre / gain configurations for selected spectrometer SNXXX
  - Redo the preprocessing of all raw ifgs recorded with SNXXX (switch on NLC corr option)
  - Redo the trace gas analysis

COCCON processing: nonlinearity correction



COCCON processing: nonlinearity correction

SN37 (2022-June-15)	Rel change NLC / no NLC
XCO2	-2.4e-4 (-0.1 ppm)
XCH4	-2.4e-4 (-0.5 ppb)

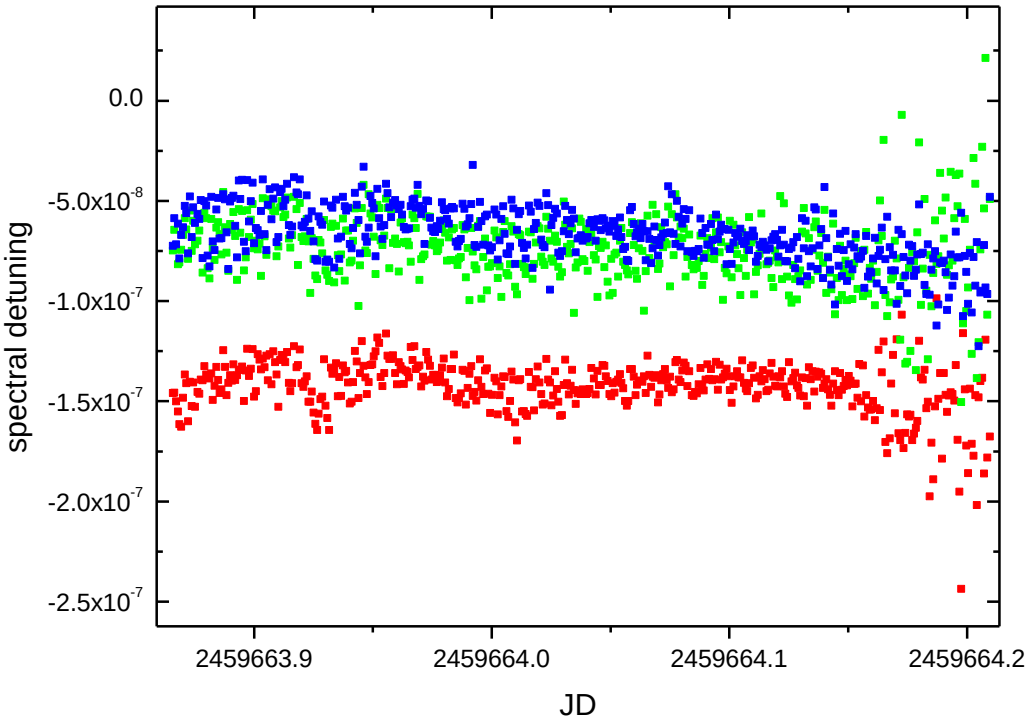
SN37 (2022-Mar-25)	Rel change NLC / no NLC
XCO2	+8.5e-5 (+0.03 ppm)
XCH4	+1.1e-4 (+0.2 ppb)

Preliminary conclusions:

- Moderate effects, but not negligible
- Corrections vary through year, during a day nearly constant (expect spurious annual cycle)
- Volunteers for code testing / evaluation of corrections required (AEMET/COCCON Spain?)
- Application would impose quite some work (characterisation of each unit required)!

COCCON processing: solar Doppler scale

- Diagnosis of residual solar Doppler scale after convergence is reached
- Performed for each existing job (variable quality), new output variable "jobXY_sol"
- Good pointing stability found for EM27/SUN FTS standard camtracker



Results from 3 different spectral fitting regions shown here.

Note: solar equatorial rotation speed ~ 2 km/s

Therefore:
1e-7 spectral detuning ~ 0.2' offset (equatorial component)

Summary

Implemented in PROFFAST operational ver 2.4

- New PREPROCESS supports data analysis for shipborne meaurements
- Calculation of daily x-section tables is accelerated

Implemented in internal beta version of PROFFAST:

- Nonlinearity correction scheme
- Residual solar Doppler analysis