Technical note on XCO_2 bias in current PROFFAST distribution

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D. Dubravica, F. Hase (darko.dubravica@kit.edu, frank.hase@kit.edu)

When working with the PROFFAST code (distributed executable generated on 10-08-2020 or later), several investigators noted a low bias in the resulting XCO_2 in the order of 0.5 ppm (Yao Té, Sorbonne Université, was the first one to point our attention to the problem – thanks so much!).

In the meanwhile, we identified the reason of the problem: the PROFFAST version generated on 10-08-2020 incorporated a bug fix (the dynamical array containing the measured spectrum was erroneously handled with a pointer offset of magnitude 1 in the invers code, this error was removed). The resulting changes in XAIR, XH_2O, XCH_4, XCH_4_S5P, and XCO were found to be negligible for practical purposes, but it was overlooked that the change in XCO_2 was in the order of 0.5 ppm.

The recent versions of PROFFAST continue to use the empirical calibration factors adjusted using the code versions predating the bug fix, so for XCO_2, a significant calibration issue when using the current version of the code results. A major revision of PROFFAST is planned in the framework of the ESA project FRM4GHG-II (will become available by end of 2021). In this new version, the currently used spectroscopic line lists will be updated and therefore the complete set of empirical calibration factors will be revised. In order to avoid confusion by distributing a further interim set of calibration factors and to avoid the need for reprocessing, we recommend the following approach:

If you use the PROFFAST version generated on 10-08-2020 or a later version, the resulting XCO_2 has a low bias. In order to remove this low bias, multiply the reported XCO_2 results in the "invparms"-table by the following airmass-dependent correction:

$$\mathbf{1.0018 - 0.001 * (SZA/90°)^2}$$

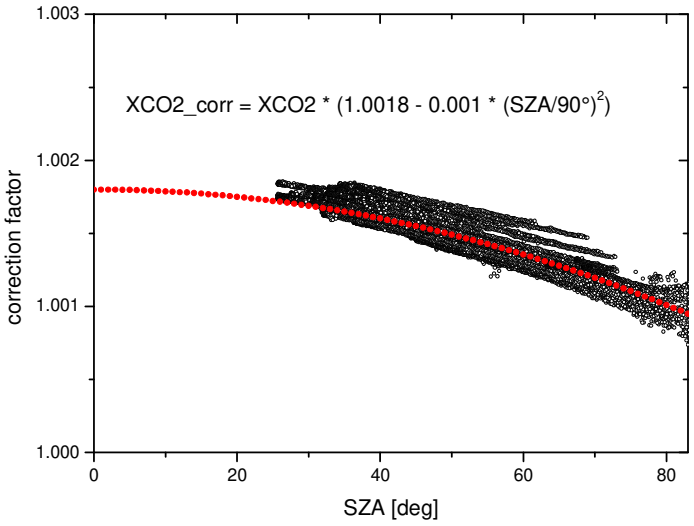

Figure: effects of suggested post-correction for XCO_2 on EM27/SUN FTIR time series recorded in Karlsruhe.