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Calibration of the EM27/SUN Instruments

This document contains a table of individual instrumental line shape (ILS) parameters for all EM27/SUN spectrometers calibrated at KIT identified by their individual serial number (SN) [1, 3]. For each instrument, a parameter set consisting of the modulation efficiency (ME) at maximum optical path difference ($\mathrm{OPD_{max}}$) and the phase error (PE) is derived from open path measurements before delivery of each spectrometer to the customer (see table 1) [2]. These parameters are required for the preprocessing of the raw data and added in the header info of the calibrated spectra (see also the demo input file and the source code of the PREPROCESS tool). Therefore, it is mandatory to replace the corresponding entries by the individual values of the instrument in the second section of the preprocessing input file (i.e. 'preprocess4.inp').

In addition, instrument-specific calibration factors $\mathrm{K_{gas}^{SN}}$ for XCO_2, XCH_4 and O_2 column amount with respect to the reference EM27/SUN spectrometer (SN37) are listed in table 3. Ideally, identical calibration factors are expected for all instruments, because the individual empirical ILS parameters were used for the trace gas retrieval. However, due to the remaining uncertainties of the ILS measurement and other possible unidentified impact factors, small deviations from the ideal unity value are found. The instrument-specific correction function is defined as:

$$\mathrm{X_{gas}^{corr}} = \mathrm{K_{gas}^{SN}} \cdot \mathrm{X_{gas}^{unc}} \ . \tag{1}$$

The column averaged dry air mole fraction $\mathrm{X_{gas}^{unc}}$ as a result of the retrieval has to be multiplied by the specific calibration factor $\mathrm{K_{gas}^{SN}}$. The tool which will generate the NetCDF datasets from the output PROFFAST ASCII tables will apply these instrument specific calibration factors (under preparation).

In addition to the instrument specific calibration factors discussed above, which aim at making data recorded with different EM27/SUN spectrometers mutually consistent, global calibrations need to be applied in order to bring COCCON data in agreement with the units used by TCCON (which are adjusted to in-situ/WMO trace gas units by using a large number of in-situ air craft profiles). For this purpose, two multiplicative corrections are applied in the framework of the PROFFAST data analysis: an air mass independent correction factor (AICF) and an air mass dependent correction factor (ADCF). The parameters for the air mass dependent and independent corrections applied for each target gas are summarized in table 4. The functional form used in PROFFAST is defined as follows:

$$\mathrm{X_{gas}}(x) = a_{\mathrm{gas}} \cdot \left\{ \frac{1 + x^4 \cdot \left(b_{\mathrm{gas}} + c_{\mathrm{gas}} \cdot x^8\right)}{1 + x_{\mathrm{ref}}^4 \cdot \left(b_{\mathrm{gas}} + c_{\mathrm{gas}} \cdot x_{\mathrm{ref}}^8\right)} \right\} \cdot \mathrm{X_{gas}^{corr}} \ , \tag{2}$$

$$\text{with} \quad x = \frac{2}{\pi} \cdot \theta \ , \quad \text{and} \quad x_{\mathrm{ref}} = \frac{2}{3} \quad \text{or} \quad \theta_{\mathrm{ref}} = \frac{\pi}{3} \quad (\equiv 60^\circ) \ .$$

Note: the neutral point of the ADCF is chosen to be 30° solar elevation (or 60° solar zenith angle). This reference value of 30° is representative for stations in the mid latitudes where most EM27/SUN spectrometers are operated. The number of measurements with solar elevation angels below this reference value is expected to be equal to the number of measurements with higher angels. By this choice, the cross-talk between the air mass dependent and independent correction can be minimized. The first parameter a_{gas} corresponds to the air mass independent

correction, the second b_{gas} and the third c_{gas} parameter accordingly to the higher order correction term for the air mass dependency. Currently, the third parameter for higher order of approximation is set to zero for all species. This part of the post-processing which is independent of the individual spectrometer is included in the PROFFAST retrieval. The parameter values listed in table 4 are reflected in the second last section of the input file 'inver10.inp'.

Table 1: Summary of the modulation efficiencies (ME) at maximum optical path difference (MOPD) and phase errors (PE) for all EM27/SUN spectromenters (SN) calibrated in Karlsruhe. The reference instrument is SN37.

SN	Date	ME	PE [rad]	SN	Date	ME	PE [rad]
29	171121	0.9862	0.0014	103	190204	0.9835	0.0042
32	140603/0715	0.9862	0.0034	104	190204	0.9819	0.0038
33	170808	0.9814	−0.0017	106	190325	0.9805	0.0020
37	140603/0715	0.9862	0.0019	109	190325	0.9835	0.0034
38	140603/0715	0.9784	0.0009	110	190326	0.9854	0.0067
39	140603/0715	0.9811	−0.0005	111	190211	0.9863	0.0007
41	140603/0715	0.9835	0.0001	112	190709	0.9861	−0.0009
42	160728	0.9752	0.0039	113	190715	0.9863	0.0042
44	170224	0.9714	−0.0019	114	190725	0.9852	0.0041
45	170225	0.9845	0.0034	115	190724	0.9837	0.0024
46	170725	0.9837	0.0024				
50	170317	0.9839	0.0023				
51	141204	0.9847	0.0017				
52	170317	0.9854	0.0048				
53	170317	0.9830	0.0025				
59	170630	0.9886	0.0029				
61	170714	0.9830	0.0013				
62	160121	0.9823	0.0053				
63	160121	0.9853	0.0011				
65	160510	0.9881	0.0024				
69	170710	0.9863	0.0030				
70	160802	0.9775	0.0056				
72	170208	0.9959	0.0030				
75	170515	0.9972	0.0041				
76	170609	1.0160	0.0007				
77	170926	0.9855	0.0016				
80	180417	0.9857	−0.0007				
81	180716	0.9823	0.0019				
82	180716	0.9841	0.0046				
83	180502	0.9853	0.0070				
84	180327	0.9862	0.0010				
85	171219	0.9876	0.0025				
86	180110	0.9830	0.0031				
88	180305	0.9832	0.0007				
91	180226	0.9836	0.0021				
92	180515	0.9806	0.0042				
94	180618	0.9792	0.0026				
95	180619	0.9805	0.0016				
96	181109	0.9850	0.0028				
97	181109	0.9852	−0.0006				
98	181109	0.9901	0.0054				
99	181106	0.9795	0.0053				

Table 2: Calibration factors for XCO_2, XCH_4 and O_2 for all investigated instruments (SN) with respect to the reference EM27/SUN spectrometer (SN37) as well as calibration dates and number of coincident measurements. Values in brackets denote percent standard deviations. PART I

SN	Dates	No. co.	K_{XCO_2}	K_{XCH_4}	K_{O_2}
29	140606/0718	490	1.0004 (0.02)	0.9997 (0.03)	1.0008 (0.03)
32	150414 − 22	1548	0.9997 (0.03)	0.9997 (0.03)	1.0004 (0.03)
33	170807/15	339	0.9991 (0.03)	0.9994 (0.04)	1.0009 (0.05)
38	150410 − 21, 160121	1609	0.9989 (0.03)	0.9997 (0.04)	0.9988 (0.04)
39	140717, 150414/15	1210	0.9992 (0.04)	0.9994 (0.04)	1.0003 (0.04)
41	140717, 150414 − 22	1877	0.9999 (0.03)	1.0002 (0.03)	0.9991 (0.03)
42	160730/0801	368	0.9978 (0.04)	1.0003 (0.04)	0.9975 (0.03)
44	170227	286	0.9979 (0.03)	0.9984 (0.03)	0.9985 (0.03)
45	170807/15	382	0.9995 (0.03)	0.9991 (0.04)	1.0008 (0.02)
46	170808/15	503	0.9993 (0.03)	0.9994 (0.03)	1.0003 (0.03)
50	150421/22	699	0.9999 (0.03)	0.9995 (0.03)	0.9995 (0.03)
51	160126/29	256	0.9995 (0.03)	0.9993 (0.03)	1.0007 (0.05)
52	150421/22	727	0.9990 (0.04)	0.9998 (0.05)	1.0002 (0.05)
53	150421/22	729	0.9987 (0.03)	1.0001 (0.03)	0.9992 (0.04)
59	160318	273	0.9998 (0.03)	0.9991 (0.03)	1.0019 (0.04)
61	151002, 170713	618	0.9993 (0.03)	0.9996 (0.04)	1.0000 (0.04)
62	160121	18	0.9988 (0.04)	0.9990 (0.02)	1.0002 (0.02)
63	160121	15	1.0003 (0.05)	1.0001 (0.05)	1.0002 (0.07)
65	160511	234	1.0005 (0.04)	0.9998 (0.05)	1.0020 (0.03)
69	160908, 170713	636	0.9994 (0.03)	0.9993 (0.03)	1.0008 (0.03)
70	160831/0906	522	0.9985 (0.02)	1.0005 (0.03)	0.9978 (0.03)
72	170215/16	433	0.9994 (0.05)	1.0001 (0.03)	0.9999 (0.04)
75	170516/17	852	0.9993 (0.03)	0.9991 (0.03)	1.0018 (0.05)
76	170608	365	0.9991 (0.04)	0.9997 (0.04)	1.0026 (0.06)
77	170927	389	0.9999 (0.03)	0.9997 (0.03)	1.0001 (0.04)
80	180418/19	835	0.999898	1.000097	1.000265
81	180718/0719/0724/0725/1018, 190225 − 0228/0322/0328/0329/0411/0415/0416/0418, 190425/0430/0619/0624 − 0628/0702 − 0705/0709/0710/0716/0717/0722 − 0725	12872	0.998625	1.000553	0.992372
82	180717 − 19	857	1.000044	1.000474	0.999273
83	180507	449	0.999583	0.999952	0.999904
84	180406/11/18/19	1681	0.999907	0.999934	1.000416
85	180124/0208/0213/0214	734	1.001819	1.002932	0.996894
86	180124/0208/0213/0214	978	1.002420	1.001521	0.997691
88	180314	205	0.999657	0.999964	1.000329
91	180228	299	0.999369	0.999965	1.000330
92	180515	25	1.000071	0.999672	1.001200
94	180620	338	1.000379	0.999454	1.001254
95	180620	317	1.000360	1.000209	0.999702
96	190213/0218/0225 − 0329/0619	3012	1.003433	1.000845	1.003081

Table 3: Calibration factors for XCO_2, XCH_4 and O_2 for all investigated instruments (SN) with respect to the reference EM27/SUN spectrometer (SN37) as well as calibration dates and number of coincident measurements. Values in brackets denote percent standard deviations. PART II

SN	Dates	No. co.	K_{XCO_2}	K_{XCH_4}	K_{O_2}
97	$190225 - 28^{(a)}$	1605	1.000253	0.999361	0.995864
98	$190218/25 - 28^{(a)}$	1771	1.001250	1.000023	0.995409
99	181107/09	294	1.000803	1.000472	1.000387
103	190205/06	530	1.000409	1.000588	0.999674
104	$190204 - 06$	788	1.000503	0.999964	1.001048
106	$190328^{(a)}$	223	1.000392	0.999279	1.002388
109	$190328^{(a)}$	194	0.999968	0.998959	1.002611
110	$190328^{(a)}$	230	0.999975	0.999665	1.001347
111	190213	344	1.000120	1.000217	0.999565
112	190709/10	581	1.000304	0.999607	0.999346
113	190716/17	959	0.999936	0.999897	0.999443
114	190724	259	1.000158	0.999975	0.998559
115	190725	525	1.000232	0.999639	0.999556

(a) alternative reference EM27/SUN spectrometer SN81 (instead of SN37)

Table 4: Parameters for the air mass dependent and independent correction function for certain target gases and microwindows (MW).

Species	MW	AICF a_{gas}	ADCF b_{gas}	ADCF c_{gas}
XH_2O	$(8353.4, 8463.1)$	0.8300	0.000	0.0
XAIR	$(7765.0, 8005.0)$	0.9737	-0.007	0.0
XCO_2	$(6173.0, 6390.0)$	0.9862	0.005	0.0
XCH_4	$(5897.0, 6145.0)$	0.9905	-0.014	0.0
XCO	$(4208.7, 4318.8)$	0.9250	0.103	0.0
$XCH_4^{(b)}$	$(4208.7, 4318.8)$	0.9727	-0.017	0.0

(b) XCH_4 S5P (Sentinel-5 Precursor)

References

[1] Gisi et al., AMT 5 (11), 2969 – 2980 (2012), doi: 10.5194/amt-5-2969-2012
[2] Frey et al., AMT 8 (7), 3047 – 3057 (2015), doi:10.5194/amt-8-3047-2015
[3] M. Frey, Dissertation (2018), doi: 10.5445/IR/1000088312