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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 (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 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 **??**. 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:

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

The column averaged dry air mole fraction X_{gas}^{unc} as a result of the retrieval has to be multiplied by the specific calibration factor 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:

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

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

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'.

The laboratory measurements for the calibration of the EM27SUN instruments as well as the calculations of the ILS parameters have been performed by:

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The ILS parameters and the scaling factors for each EM27/SUN instrument are summarized in the subsequent tables 1, 2, and 3.

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 SN037.

SN	Date	ME	PE [rad]	SN	Date	ME	PE [rad]
29	171121	0.9862	0.0014	103	190204	0.9835	0.0042
32	140715	0.9862	0.0034	104	190204	0.9819	0.0038
33	170808	0.9814	−0.0017	106	190325	0.9805	0.0020
37	140715	0.9862	0.0019	109	190325	0.9835	0.0034
38	140715	0.9784	0.0009	110	190326	0.9854	0.0067
39	140715	0.9811	−0.0005	111	190211	0.9863	0.0007
41	140715	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	116	190930	0.9875	0.0044
50	170317	0.9839	0.0023	117	191022	0.9791	0.0038
51	141204	0.9847	0.0017	118	191111	0.9861	0.0071
52	170317	0.9854	0.0048	119	191101	0.9826	−0.0007
53	170317	0.9830	0.0025	121	191119	0.9830	0.0085
59	170630	0.9886	0.0029	122	191119	0.9899	0.0009
61	170714	0.9830	0.0013	126	191213	0.9876	0.0019
62	160121	0.9823	0.0053	127	191211	0.9816	0.0039
63	160121	0.9853	0.0011	128	191211	0.9873	0.0006
65	160510	0.9881	0.0024	130	191217	0.9853	0.0037
69	170710	0.9863	0.0030	131	200120	0.9882	0.0007
70	160802	0.9775	0.0056	132	200116	0.9853	−0.0008
72	170208	0.9959	0.0030	134	200317	0.9902	0.0049
75	170515	0.9972	0.0041	138	200702	0.9893	0.0056
76	170609	1.0160	0.0007	139	210125	0.9857	0.0019
77	170926	0.9855	0.0016	140	210205	0.9870	0.0036
80	180417	0.9857	−0.0007	141	210212	0.9842	0.0041
81	180716	0.9823	0.0019	142	200814	0.9960	0.0047
82	180716	0.9841	0.0046	143	201110	0.9888	0.0021
83	180502	0.9853	0.0070	144	201113	0.9877	−0.0002
84	180327	0.9862	0.0010	145	210104	0.9867	0.0018
85	171219	0.9876	0.0025	146	210104	0.9889	0.0038
86	180110	0.9830	0.0031	147	210306	0.9880	0.0037
88	180305	0.9832	0.0007	149	210305	0.9884	−0.0006
91	180226	0.9836	0.0021	150	210401	0.9866	−0.0055
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
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

(*a*) alternative reference EM27/SUN spectrometer SN081 (instead of SN037)

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}
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	340	0.999786	1.000065	1.000655
116	191014	286	0.999973	0.999371	1.000569
117	191031	263	1.000220	1.000068	0.999669
118	191122	52	1.000168	0.999313	1.001487
119	191122	55	0.999635	0.999514	1.000334
121	191130	242	0.999797	0.999669	0.998840
122	191130	165	0.998723	0.999057	1.001092
126	191216	160	0.999952	0.999769	1.000174
127	191210	268	1.000392	1.000030	0.999681
128	191210	256	1.000387	1.000129	0.999486
130	191229	186	1.000058	1.000334	0.998489
131	200121	296	1.000188	0.999311	1.001412
132	200115	277	0.999925	1.000205	1.000436
134	200318	251	1.000163	0.999854	1.000163
138	200707	207	1.000141	0.999983	1.000273
139	210214	362	0.999958	0.999314	1.000810
140	210214	360	0.999945	0.999455	1.001139
141	210214	356	1.000065	0.999534	1.000802
142	200820	79	1.000226	0.998703	1.002544
143	201118	239	1.000138	0.999977	0.999123
144	201118	213	0.999540	1.000513	0.997910
145	210115	270	1.000182	1.000538	0.998224
146	210111	347	1.000241	0.999676	1.000045
147	210306	247	1.000305	0.999965	1.000682
149	210306	248	1.000296	0.999919	1.000607
150	210331	322	1.000162	1.000079	0.999991

(*a*) alternative reference EM27/SUN spectrometer SN081 (instead of SN037)

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
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[3] M. Frey, Dissertation (2018), doi: 10.5445/IR/1000088312