3.6 Uncertainty discussion

Measurements are affected by three types of error sources: random effects, known and unknown systematic effects. Random effects result in a measurement to measurement variability and can be quantified by the standard deviation. Known systematic effects should not simply be encompassed by increasing the estimated uncertainty, according to the Joint Committee for Guides in Metrology (JCGM, 2008) recommendations. They rather should be corrected and the uncertainty in the correction included in the total uncertainty of the corrected quantity. The total uncertainty is calculated as the sum in quadrature of random effects and the uncertainty of the corrected known systematic effects. Unknown systematic effects reveal in comparison to independent measurements and can be corrected against a calibration standard, such as the WMO standards, the objective of this paper.

3.6.1 Uncertainty of FTS-derived DMFs

FTS measurements are known to be mainly affected by the following systematic effects. Firstly the a priori profiles can be wrong due to false estimations of the temperature, pressure or water vapour profiles. Furthermore the volume mixing ratio shape of the a priori profiles can be wrong. Secondly the sun tracker pointing at the middle of the sun can be offset. Thirdly the instrumental line shape (ILS) can be distorted due to shear or angular misalignment of the instrument or field of view (FOV) failure (Wunch et al., 2011). The calculation of X_{CO_2} by Equation 1 reduces some of the effects that are common to both gases (solar tracking pointing errors, zero level offsets, ILS errors or surface pressure measurement errors).

Furthermore it is known that the X_{CO_2} exhibit an airmass-dependency, resulting in 1 $\%$ larger X_{CO_2} at low solar zenith angeles (SZA) than at high SZA. This dependency is removed in the standard GFIT retrieval by a single empirical correction (Section 3.1). A quantification of realistic perturbations of the a priori profile, the tracking and the ILS was done by Wunch et al. (2011). It could be estimated that the X_{CO_2} in total would be affected by 0.18 $\%$ for low SZA (20°) and 0.13 $\%$ for high SZA (70°) .

Within the IMECC campaign, potential systematic effects introduced by the a priori profiles were eliminated by using the assembled aircraft profiles as a priori profiles (Section 3.1). Concerning the quality of the solar tracking, a suitable indicator is the pointing error, which is the deviation from pointing at the middle of the sun and can be estimated by the Doppler Shift. The ILS is regularly monitored in all TCCON FTS instruments (Section 3.1) and misalignments could further be seen in the fitting residuals by characteristic artifacts. All FTS instruments and their solar tracker were optimized prior the IMECC campaign, and hence systematic effects by the pointing error and the ILS were minimized.

One known source, systematically affecting FTS measurements, was not diminished prior the campaign or is taken care of in the retrieval. Messerschmidt et al. (2010) showed that collocated FTS instruments agree within 0.07 $\%$, but only after correcting for a systematic effect introduced by a mis-sampling of the internal reference laser provided in the commercially available FTSs. Briefly, a periodic laser mis-sampling leads to so called ghosts (artificial spectral lines), which are mirror images of the original spectral lines. The influence of the ghosts on the retrieved X_{CO_2} was quantified as a function of the ghost and parent line intensities, called the ghost/parent line ratio (GPR). For a typical GPR, the retrieved X_{CO_2} is affected by about 1 ppm. Therefore, a correction scheme was introduced for solar measurements afflicted with ghosts (Messerschmidt et al., 2010). The effect of the retrieved X_{CO_2} was quantified and this correction applied to all measurements during the IMECC campaign.

The Messerschmidt et al. (2010) correction scheme does not predict the sign of the ghosts, which means that it is ambiguous as to whether the ghosts lead to an over- or an underestimation of the retrieved X_{CO_2}. For three of the FTS instruments (BIK, BRE, ORL), this sign was inferred from the side-by-side measurements detailed by Messerschmidt et al. (2010). For the Garmisch and Karlsruhe FTS instruments, the ghosts were minimized prior to the aircraft campaign and did not introduce a large systematic effect. The Jena instrument could not be corrected prior to the aircraft campaign, and had significant ghosts, which affected the retrievals. The results suggest an over-estimation of X_{CO_2}. However, as we cannot be sure of the sign, we investigate two 'worst-case' scenarios in calculating the scaling factors for the FTS relative to the in-situ profile in Section 4. These correspond to all ghosts (Table 3) leading to an (a) under- and (b) over-estimation of the retrieved X_{CO_2}. The difference between these scenarios is used to check the correction of the systematic effect introduced by the ghost correction scheme in the calculation of scaling factors.

One further source lead to systematic effects: Due to poor weather in Jena and Bremen, not all overpasses could be carried out at the same time as the FTS data were measured (BRE_1, JEN_3, JEN_4). To account for a delay of two hours in all three cases, the expected variation due to the diurnal CO_2 cycle was accounted for as a systematic effect. At both sites, the magnitude of the diurnal cycle was estimated from the trend of the FTS measurements on the same day. The diurnal cycle was calculated for BRE_1 by the trend of the FTS data taken for a 2 hour time period prior to the overpass and for JEN_3 and JEN_4 by the trend of the FTS data measured for a 2.5 hour time period after the overpass. The trends were estimated with the FTS data that met the filter criteria introduced in Section 3.1 and extrapolated to the overpass time. On-site in-situ measurements showed for the extrapolated time period in Jena a variability of $\pm$ 0.5 ppm and no significant trend that indicate further influence e.g. from local pollution or

Table 3. Systematic effects due to ghosts and a time delay between the overpass and FTS measurements and the uncertainty sources contributing to the total uncertainty of the FTS measurements. The total uncertainty accounts for the FTS measurements variability during the overpasses, an uncertainty in the estimation of the expected variation due to the diurnal cycle and the uncertainty in the ghost estimation, according to Messerschmidt et al. (2010).

code	**systematic effects** [ppm] applied correction of		**uncertainties** [ppm]			
	ghosts	time delay	ghosts	time delay	overpass variability	**total**
BIK_1	-0.27	-	0.05	-	0.12	0.13
BIK_2	-0.27	-	0.05	-	0.13	0.14
BIK_3	-0.27	-	0.05	-	0.19	0.20
BIK_4	-0.27	-	0.05	-	0.19	0.20
BRE_1	+0.31	+0.07	0.06	0.01	0.41	0.41
BRE_2	+0.31	-	0.06	-	0.38	0.39
GAR_1	+0.06	-	0.02	-	0.35	0.35
JEN_1	-1.63	-	0.16	-	0.35	0.39
JEN_2	-1.63	-	0.16	-	0.35	0.39
JEN_3	-1.63	+0.37	0.16	0.03	0.26	0.31
JEN_4	-1.63	+0.30	0.16	0.03	0.26	0.31
KAR_1	-0.12	-	0.04	-	0.35	0.35
ORL_1	+0.38	-	0.08	-	0.33	0.34
ORL_2	+0.38	-	0.08	-	0.34	0.35
ORL_3	+0.38	-	0.08	-	0.40	0.41
ORL_4	+0.38	-	0.08	-	0.38	0.39

changing meteorological conditions. For Bremen no on-site in-situ measurements exist. The BRE_1, JEN_3, JEN_4 data are not included in the calculation of the calibration factor, due to the remaining lack of information during the overpasses, but the results will be discussed in Section 4.2.

Random effects, such as noise and variations in the solar tracker and instrument performance, are quantified by the measurement to measurement variability during the overpasses.

The total uncertainty for the FTS data is the sum in quadrature of the contributing standard uncertainties: the standard deviation about the mean during the overpass, the standard uncertainty of the ghost estimation and the standard uncertainty of the diurnal cycle estimation. Table 3 summarizes the magnitude of the systematic corrections, the uncertainties and the total uncertainty for all overpasses.

3.6.2 Uncertainty of the assembled in-situ data

The uncertainty of the assembled in-situ data is derived from the uncertainty of the aircraft measurements, the uncertainties in extrapolating the profiles and the usage of contemporary profiles (Table 4).

The GFIT a priori CO_2 profiles are used to extend the in-situ data above the tropopause, as explained in Section 3.4. Thus a typical profile of mean age (Andrews et al., 2001) above the local tropopause is used to calculate the lag of stratospheric CO_2 values with respect to mean tropospheric values. Furthermore a decrease of the seasonal cycle with altitude is taken into account. Seasonally resolved aircraft measurements during the SPURT project (Engel et al., 2006) revealed that the seasonal cycle in the lowermost stratosphere (i.e. the region of the stratosphere between the local tropopause and the 380K isentrope) is not only attenuated with increasing vertical distance to the local tropopause but is also shifted with respect to the troposphere (Hoor et al., 2004; Bönisch et al., 2008, 2009; Hintsa et al., 1998). The seasonal cycle magnitude can be as large as 3 ppm at the mid latitude tropopause and decreases to about half of that value at about 50 K potential temperature above the local tropopause. The amplitude and timing of the seasonal cycle at the tropopause is captured quite well in the a priori profiles with a maximum in May. The variability in this area is, however, very high, especially when using pressure coordinates. Therefore a conservative uncertainty estimate is used by assuming that the CO_2 seasonal cycle in the lowermost stratosphere can not be correctly represented and that this seasonal cycle leads to an additional uncertainty of the CO_2 a priori profile of about 2 ppm, that is a typical amplitude of the seasonal cycle in the lowermost stratosphere. This uncertainty is independent of contributions from the absolute uncertainty of the mean age profile, that is estimated to be about 0.3 ppm (Wunch et al., 2010). The total uncertainty of the stratospheric CO_2 values is thus estimated as the sum in quadrature and on the order of 2.02 ppm.

For some overpasses, the profiles could not be measured up to the tropopause. If no contemporary aircraft profile was available, the upper troposphere was filled with the highest aircraft measurement; e.g. as clearly seen in Figure A2. The CO_2 variability in the upper troposphere, measured at the European TCCON sites, is within 2 ppm and applied as uncertainty for the filling. If a contemporary aircraft profile was available, it was used to estimate the profile above the last aircraft measurement (Figure A1,A3, A4). It is assumed that the profile can therewith be better estimated than by using the highest aircraft measurement and an uncertainty of 1.5 ppm is assigned.

For the aircraft data, the standard uncertainty provided by the post-flight analysis at the MPI-BGC's lab was applied. The uncertainties given for the mixing ratios contain uncertainties from extension with the lowest aircraft measurement to the surface pressure, as well as from interpolation across missing values (e.g. due to instrument calibration periods). Also included is the statistical uncertainty from sampling only a limited number of seconds at each pressure interval. In addition, an uncertainty related to the calibration of the standard gases (working tanks) against WMO primary gases

Table 4. Contributing uncertainties to the total uncertainty of the assembled in-situ data. The total uncertainty is calculated by the sum in quadrature of the weighted fraction in terms of pressure with respect to the completed in-situ profile.

Uncertainties contributing to the total uncertainty	[ppm]
stratospheric extrapolation	2.02
missing tropospheric values	2.00
usage of contemporary profile	1.50
mean aircraft profile	0.11

is added. The mean standard deviation for the IMECC campaign aircraft profiles is 0.11 ppm. The total uncertainty is calculated from the sum in quadrature of these contributing uncertainties weighted by their relative contribution to the completed profile in terms of pressure.

Due to poor weather conditions a profile was not flown above the Karlsruhe TCCON site. Aircraft measurements were, however, recorded during a stop-over 50 km to the south of the site. The Karlsruhe data are therefore treated similarly to the other overflights, but because of these exceptional circumstances, they are not included in the calculation of the calibration factor. They will be discussed in Section 4.2.

The resulting uncertainties for the FTS measurements and for the integrated column-averaged assembled aircraft CO_2 profiles are listed for all overpasses in Table 5.

Table 5. The IMECC campaign results: The code of each overpass, the type, the solar zenith angle (SZA), the aircraft ceiling/- floor, spiral range, nearest distance, number of FTS measurements during the overpass, and the column-integrated CO_2 abundances measured by in-situ instrumentations and FTS are given.

code	type	SZA [°] (min-max)	aircraft ceiling [km]	aircraft floor [m]	spiral [km] (ceiling,width)	nearest distance [km]	number of FTS data	FTS [ppm]	aircraft [ppm]
BIK_1	descent	56.2-61.1	11.5	500	(5,10)	0	65	378.3 ± 0.1	382.6 ± 0.1
BIK_2	ascent	56.2-61.1	8	500	(3,5)	0	67	378.3 ± 0.1	382.5 ± 0.2
BIK_3	descent	66.8-72.4	8	800	(5,8)	0	35	378.1 ± 0.2	382.5 ± 0.2
BIK_4	ascent	66.8-72.4	10.5	800	(5,10)	0	35	378.1 ± 0.2	382.5 ± 0.1
BRE_1	descent	58.0-75.5	13	500	(6,10)	0	30	379.1 ± 0.4	383.7 ± 0.1
BRE_2	descent	59.5-62.8	13	500	(10,10)	0	37	378.7 ± 0.4	383.5 ± 0.1
GAR_1	descent	53.9-62.3	12.5	1500	(7,15)	5	19	379.6 ± 0.4	384.1 ± 0.1
JEN_1	descent	59.0-63.8	12.5	800	(7,10)	0	8	379.7 ± 0.4	383.7 ± 0.1
JEN_2	ascent	59.0-63.8	8	800	-	0	8	379.7 ± 0.4	383.8 ± 0.2
JEN_3	descent	59.9-61.7	12.5	500	(9,15)	0	7	380.0 ± 0.3	384.1 ± 0.1
JEN_4	ascent	59.9-61.7	12.5	500	-	0	7	380.0 ± 0.3	384.1 ± 0.1
KAR_1		54.2-64.3	7	200	-	10	26	380.8 ± 0.4	384.6 ± 0.2
ORL_1	descent	68.9-83.6	11.5	700	(9,15)	30	45	380.1 ± 0.3	384.2 ± 0.1
ORL_2	ascent	68.9-83.6	7	700	(3,5)	0	45	380.0 ± 0.4	384.2 ± 0.2
ORL_3	descent	51.8-52.5	11	700	(8,30)	12	10	380.3 ± 0.4	384.1 ± 0.1
ORL_4	ascent	51.8-52.5	8	700	(5,5)	0	10	380.3 ± 0.4	384.2 ± 0.2