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Supplement of

Airborne remote sensing and in situ measurements of atmospheric CO₂ to quantify point source emissions

Thomas Krings et al.

Correspondence to: Thomas Krings (thomas.krings@iup.physik.uni-bremen.de)

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Details about the in-situ fluxes from a variety of methods; using the variations for error estimates

day_source	S4: Fimmersdorf	S3: Neurath_old	S2: Neurath_new	S1: Niederaussem	percentage measured (rest was extrapolated)	different variations of our linear method						average	minima	maxima	relative error estimate	by Kriging		extreme to unrealistic assumptions			remarks		
						200 x 100 fb	flux 2	200 x 100	200 x 100 lb	100 x 100	200 x 200					Kriging	Kriging 2	200 x 100 ce	bulk average	bulk average 2			
15_RWE_cluster_total	X	X	X	X	86%	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	Mt/a	lower limit
15_RWE_cluster_3 (all except S4)		X	X	X	80%	38.7	42.7	40.3	40.3	34.3	42.1	39.7	34.3	42.7	10%	26.20	43.90	50.00	36.47	41.41		lower limit	
15_RWE_Frimmersdorf isolated below 450 m	X				55%	1.6	2.7	1.3	1.5	1.4	1.7	1.7	1.3	2.7	41%			2.25	1.21	2.72		clear small plume	
15_RWE_Neurath old isolated below 600 m		X			57%	17.6	18.0	13.3	17.3	17.4	27.3	18.5	13.3	27.3	38%			25.14	29.26	28.40		single crossing	
15_RWE_Niederaussem				X	90%	26.2	26.6	25.8	26.2	26.1	22.0	25.5	22.0	26.6	9%	21.50	23.50	30.96	26.31	24.78		high data density	
23_Weisweiler					100%	18.4	16.3	18.1	18.3	18.3	20.9	18.4	16.3	20.9	13%	15.40	17.50	16.24	27.80	25.40		ideal single source on other day	

reference calculations with the most plausible parameters

average from the six variations of our method, as explained below

relative deviations from (max-min)/2

Explanation and caption for primary data, including the comparison with the older version from 2016

This table is summarizing different methods for flux calculations, applied to different sources in the RWE cluster as measured on 15 Aug 2012.

The plume Weisweiler eight days later was included as a reference case under almost ideal conditions (good coverage perpendicular to the wind, no extrapolation; however low average wind speed of only 3.7 m/s).

Caption for the columns see in the next red frame below.

day_source and S1 to S4	day in August 2012 and names of the sources
percentage measured	contribution of layers with measurements; the rest of the fluxes is extrapolated down to the surface and up to the assumed stable layer
200 x 100 fb	gridding with 200 x 100 m (horizontal x vertical) with fixed background concentration; individual flux calculations at each measurement point (5 Hz)
flux 2	the same gridding and background, but, the fluxes were calculated after the gridding as wind x mass
200 x 100	the same gridding, but, the background concentrations were calculated as the minimum concentration per layer
200 x 100 lb	the same as above, but this stratified background concentration was limited
100 x 100	finer grid; the rest is like the reference calculation according to 200 x 100 fb
200 x 200	coarser grid; the rest is like the reference calculation according to 200 x 100 fb
average	the average from all the standard methods listed above (without the methods listed after the error estimates)
minima	the minimum fluxes from the various methods
maxima	the maximum fluxes from the various methods
relative error estimate	half of the maxima minus the minima divided by the average
Kriging	the local fluxes interpolated by Kriging; as can be seen from the results and even better from the fields, they are too smooth, tending to underestimate the fluxes
Kriging 2	same as 'flux 2', but with wind and mass after Kriging. Also these results are less plausible than obtained by our standard method (see difference Kriging-Kriging2)
200 x 100 ce	the same gridding and background as 200 x 100 fb, but, the extrapolations to the surface and to the top were done with constant concentrations, which is extreme
bulk average	the pointwise fluxes averaged without any interpolation, multiplied with the total cross section. This is without any assumptions about the shape of the plume!
bulk average 2	the flux resulting from multiplying the averaged wind with the averaged excessive mass. See the text in the paper for a statement about these bulk averages.

ID	Deriving individual source contributions from sums and differences															
A	Niederaussem (S1) directly measured				X		26.2						25.5	22.0	26.6	9%
B	cluster 3 (all except S4)		X	X	X		38.7						39.7	34.3	42.7	10%
C	Niederaussem separated in cluster 3				X		27.6						23.5	17.8	32.8	32%
D	Neurath old separated in cluster 3		X				16.8						16.8	13.3	20.8	22%
E	Neurath new separated in cluster 3			X			7.3						7.3	3.9	11.3	50%
F	Frimmersdorf separated from cluster total	X					1.6						1.7	1.3	2.7	41%
G	cluster total measured directly	X	X	X	X		53.4						51.9	50.0	55.4	5%
H	cluster 3 plus S4	X	X	X	X		40.3						41.4	35.6	45.3	12%
I	missed in cluster_3 (added for B to E)						13.1						10.5	4.7	19.8	72%
J	A+D+E+F	X	X	X	X		51.9						51.3	40.6	61.3	20%
K	(G+J)/2 and min, max for errors	X	X	X	X		52.6						51.6	50.0	61.3	11%

Sums and differences, listed as cases A to K:

	A, F, G, and the sum (B = A+D+E) were directly measured. For the latter (called 'cluster 3: all except S4'), the three contributions for A, D, and E were estimated graphically on the cross section (figure 8). In sums and differences, the ranges were calculated using the extrema (minima or maxima). The uncertainty of the graphical separation was done by a wide variation of the assumptions (e.g. percentage overlap of the plumes 20..80 %). These error estimates are rather conservative.
	Description and Comments to the 11 Cases:
A	direct measurement that should be quite accurate, i.e. no evident over- or underestimation. This is the most robust number in the data set. However, also here, extrapolation from 1100 m to 1300 m was necessary, adding to the overall uncertainty as presented in table 3 of the paper.
B	cluster 3 copied from the table of the primary measurements
C	separated graphically in the cross section 'cluster 3' (fig. 8), where the three sources C, D, and E can be seen, but, not sharply discriminated. For the error estimate, the split was varied between extreme assumptions.
D	See C and the graph of the cross-section (fig. 8)
E	See C and the graph of the cross-section (fig. 8)
F	directly measured; this is the most significant change compared to the first version of the paper. Based on the information, that this source was rather weak, it was possible to see, that indeed only a small plume below 450 mAMSL was visible (fig. 7). This plume is marked on the new cross-section of the total cluster, and was inspected separately in a higher resolution (100 x 100 m ²)
G	directly measured, with a certain risk, that the top of the plume (linearly extrapolated to flux zero on 1300 mAMSL) is underestimated. It is therefore a lower limit of the flux.
H	'cluster 3' plus Frimmersdorf (F) is now better than before, and rather an underestimation. The underestimation can be estimated by the difference I, which was used before calculating the scenarios C, D, and E
I	The difference between two methods to obtain the total emission. This difference was used to adjust G before splitting into C, D, E.
J	Checksum of the individual sources. After the adjustments explained above, this is well in agreement of the directly measured total emission of the cluster. However, the minimum and maximum has a wider range.
K	Because G is clearly a lower limit of the total emission, the minimum is taken from there, and not from J. On the other hand, the maximum of J is the upper limit of the total emission.