Supplementary material to: Quantitative sampling and analysis of trace elements in atmospheric aerosols: impactor characterization and Synchrotron-XRF mass calibration

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1 Supplementary Material

1.1 Scatterplots

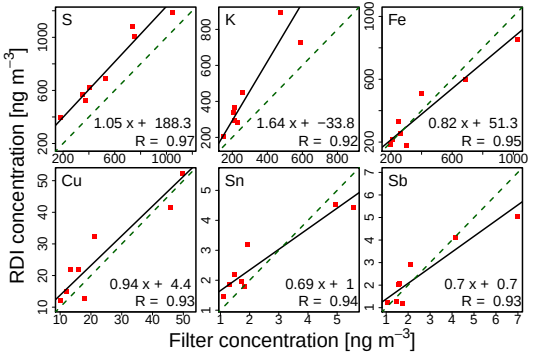

Fig. 1. Correlation scatterplots of PM_{10} RDI versus filter concentrations (both in $\mathrm{ng\ m^{-3}}$) for the Zürich winter campaign 2008/09 for S, K, Fe, Cu, Sn and Sb. Each data point corresponds to one day, i.e. one filter value and the mean of 12 2h-RDI values. A Deming orthogonal regression (not forced to have an intercept of zero) is applied to the data, since both methods are subject to measurement uncertainties. Cornbleet et al. (1979) stated that an orthogonal regression should be chosen in cases, where also the independent (x-axis) variable has a certain imprecision. Furthermore, outliers should not be included if their vertical distance from the regression line is larger than four times the standard error of the estimate. The Deming regressions were performed with the MethComp Package in the software R (see R Development Core Team, 2008) and one outlier was excluded from the data set. The obtained slope and intercept as well as the Pearson correlation coefficient are depicted in each plot.

1.2 Averaged Values

Table 1. Comparison of average mass concentrations: the first two columns present mean values of elements measured by PM_1 and PM_{10} high-volume filters compared to the same elements measured with the RDI. PM_1 daily filter samples were taken every day in the period from 30 November 2008 till 17 December 2008 and analyzed for the following elements (a): Al, P, S, K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Rb, Sr, Zr, Cd, Sn, Sb, Ba and Pb. PM_{10} daily filter samples were taken every second day in the period from 1 till 17 December 2008 and analyzed for the following elements (b): Al, P, S, Cl, K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Rb, Sr, Zr, Mo, Cd, Sn, Sb, Ba and Pb. In addition, average values for all data points throughout the whole campaign as well as the same period excluding New Year's Eve (NYE, 31 December 2008 15:00 LT to 1 January 2009 05:00 LT) are shown. The third column lists the average values for the whole range of elements, which can be detected by the RDI-SR-XRF method (c): Al, Si, P, S Cl, K Ca, Ti, Cr Mn, Fe, Co, Ni, Cu, Zn, Sr, Zr, Mo, Cd, Sn, Sb, Ba and Pb. The last two columns give averaged values for quasi-continuously monitored PM_{10} mass concentrations as well as averaged $PM_{2.5}$ and PM_{10} mass concentrations from daily filter analysis. Values marked with an asterisk (*) are averaged only for days in 2008 (28 November till 31 December).

PM_1	Filter (a)	RDI (a)	all RDI elements (c)	PM_1 cont.	PM_1 daily
Filter period	0.64	0.68	0.69	-	-
Whole camp.	-	1.99	2.02	-	-
Period w/o NYE	-	1.67	1.68	-	-
$PM_{2.5}$	Filter (NA)	RDI (NA)	all RDI elements (c)	$PM_{2.5}$ cont.	$PM_{2.5}$ daily
Whole camp.	-	-	3.52	-	-
Period w/o NYE	-	-	3.08	-	21.19*
PM_{10}	Filter (b)	RDI (b)	all RDI elements (c)	PM_{10} cont.	PM_{10} daily
Filter period	2.7	2.55	2.78	20.56	20.61
Whole camp.	-	5.09	5.3	25.23	-
Period w/o NYE	-	4.58	4.79	24.64	24.96*

References

Cornbleet, P. J., and Gochman, N.: Incorrect Least-Squares Regression Coefficients in Method-Comparison Analysis, Clin. Chem., 25 (3), 432, 1979.

R Development Core Team: R: A language and environment for statistical computing. R Foundation for Statistical Computing, http://www.R-project.org, 15.05.2010, Vienna, Austria, ISBN 3-900051-07-0, 2008.