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Characterizing water vapour concentration dependence of commercial cavity ring-down spectrometers for continuous on-site atmospheric water vapour isotope measurements in the tropics

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S1 IRMS methodology

The $\delta^{2}H$ and $\delta^{18}O$ measurements were done on a Delta^{+}XL isotope ratio mass spectrometer coupled to a high-temperature conversion reactor (HTC) via a ConFloIII. The analysis method is described in Gehre et al. (2004). A daily sequence consisted of the DI1 or DI2 water samples, an in-house reference standard www-j1 (Willi Working Water-Jena1; $\delta^{2}H$: -66.45 ± 1.0 ‰, $\delta^{18}O$: -9.78 ± 0.10 ‰), an in-house scaling standard BGP-j1 (Brand Greenland Precipitation-Jena1; $\delta^{2}H$: -187.94 ± 1.0 ‰, $\delta^{18}O$: -24.46 ± 0.10 ‰), and an in-house quality control RWB-j1 (ReinstWasser Brand-Jena1; $\delta^{2}H$: -1 ± 1.0 ‰, $\delta^{18}O$: 7.8 ± 0.10 ‰). The daily average standard deviation of www-j1 was better than 0.16 ‰ (n = 44) for $\delta^{18}O$, and better than 0.7 ‰ (n = 41) for $\delta^{2}H$ measurements. All in-house standards are regularly calibrated and checked against the international IAEA standards VSMOW2 and SLAP2. Thus the DI1 and DI2 isotope values are given on the VSMOW/SLAP scale.

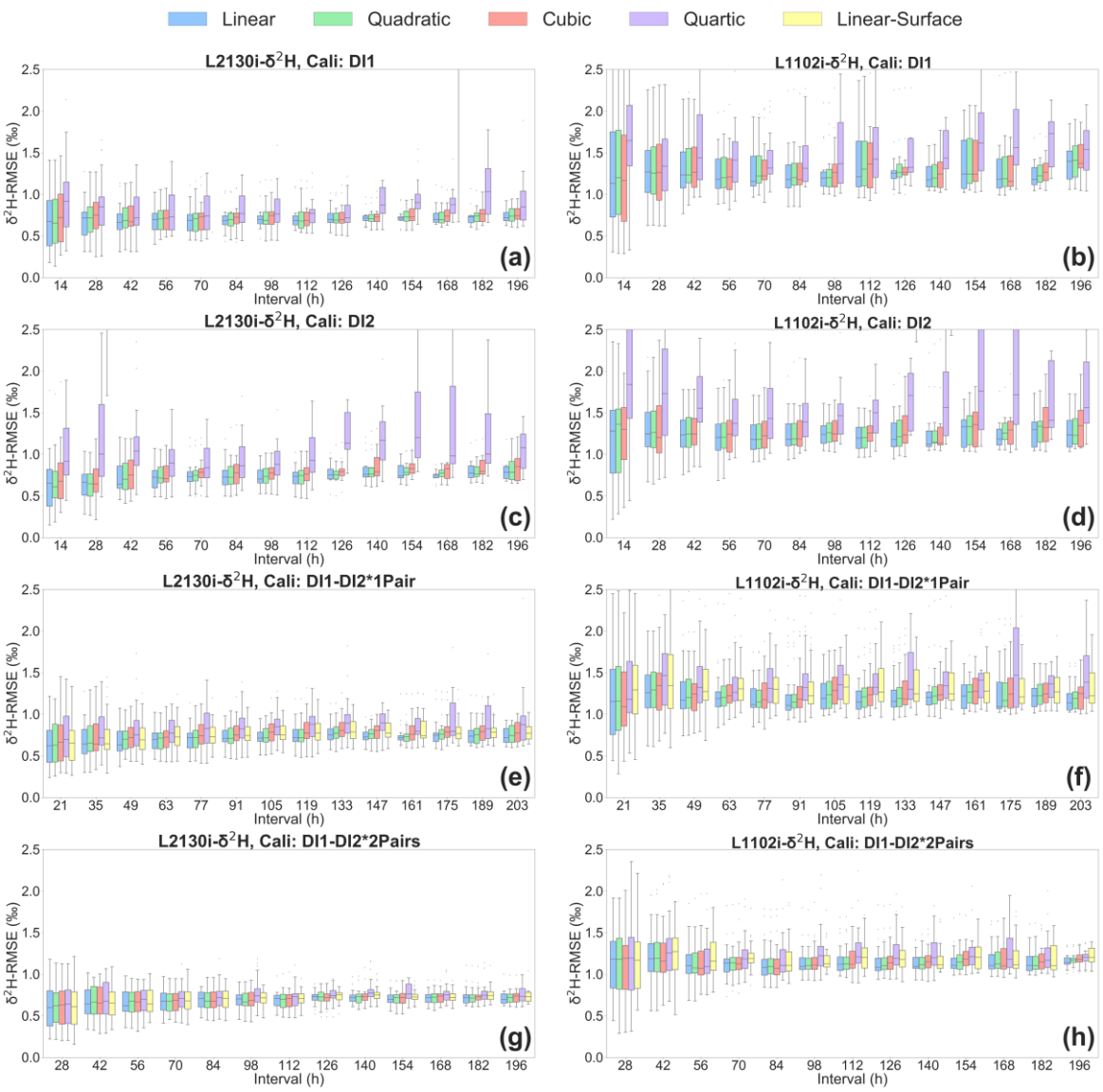

Figure S1 Boxplots of root mean square error (RMSE) of δ^2H, derived from calibrating [H_2O]-dependence of δ^2H measurements by each of five fitting methods (i.e., linear, quadratic, cubic, quartic, linear surface fitting methods) for each of four calibration strategies: DI1, DI2, DI1-DI2*1Pair, DI1-2*2Pairs. Boxplots of (a) L2130's and (b) L1102's δ^2H RMSE for the DI1 strategy, depending on interval length (i.e., the time period used for calibrating [H_2O]-dependence). Boxplots of (c) L2130's and (d) L1102's δ^2H RMSE for the DI2 strategy, depending on interval length. Boxplots of (e) L2130's and (f) L1102's δ^2H RMSE for the DI1-DI2*1Pair strategy, depending on interval length. Boxplots of (g) L2130's and (h) L1102's δ^2H RMSE for the DI1-2*2Pairs strategy, depending on interval length. The procedure for assessing [H_2O]-dependence uncertainties (= RMSE) is described in section 2.3.

References

Gehre, M., Geilmann, H., Richter, J., Werner, R. A. and Brand, W. A.: Continuous flow $^{2}H/^{1}H$ and $^{18}O/^{16}O$ analysis of water samples with dual inlet precision, Rapid Communications in Mass Spectrometry, 18(22), 2650–2660, doi:10.1002/rcm.1672, 2004.