

Abstract

Several initiatives are currently emerging to observe the exchange of energy and matter between the earth's surface and atmosphere standardized over larger space and time domains. For example, the National Ecological Observatory Network (NEON) and the Integrated Carbon Observing System (ICOS) will provide the ability of unbiased ecological inference across eco-climatic zones and decades by deploying highly scalable and robust instruments and data processing. In the construction of these observatories, enclosed infrared gas analysers are widely employed for eddy-covariance applications. While these sensors represent a substantial improvement compared to their open- and closed-path predecessors, remaining high-frequency attenuation varies with site properties, and requires correction. Here, we show that the gas sampling system substantially contributes to high-frequency attenuation, which can be minimized by careful design. From laboratory tests we determine the frequency at which signal attenuation reaches 50 % for individual parts of the gas sampling system. For different models of rain caps and particulate filters, this frequency falls into ranges of 2.5–16.5 Hz for CO₂, 2.4–14.3 Hz for H₂O, and 8.3–21.8 Hz for CO₂, 1.4–19.9 Hz for H₂O, respectively. A short and thin stainless steel intake tube was found to not limit frequency response, with 50 % attenuation occurring at frequencies well above 10 Hz for both H₂O and CO₂. From field tests we found that heating the intake tube and particulate filter continuously with 4 W was effective, and reduced the occurrence of problematic relative humidity levels (RH > 60 %) by 50 % in the infrared gas analyser cell. No further improvement of H₂O frequency response was found for heating in excess of 4 W. These laboratory and field tests were reconciled using resistor-capacitor theory, and NEON's final gas sampling system was developed on this basis. The design consists of the stainless steel intake tube, a pleated mesh particulate filter, and a low-volume rain cap in combination with 4 W of heating and insulation. In comparison to the original design, this reduced the high-frequency attenuation for H₂O by $\approx 3/4$, and the remaining cospectral correction did not exceed 3 %, even at a very high relative humidity (95 %). This

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The EC technique is used worldwide across numerous ecosystems to directly measure the exchange of momentum, energy and atmospheric trace gases between the earth's surface and atmosphere (Aubinet et al., 2012; Baldocchi et al., 1988; Swinbank, 1951). A typical EC system consists of a fast-response 3-D sonic anemometer for wind measurements, and an infrared gas analyser (IRGA) for H₂O and CO₂ measurements, often with fundamental response times of ≤ 0.1 s. However, additional infrastructure such as the IRGA gas sampling system (GSS) can decrease frequency response. As a result, high-frequency spectral corrections can exceed several 10 %, in particular for water vapour (e.g., Ammann et al., 2006; Fratini et al., 2012; Ibrom et al., 2007). Active testing and research on optimizing GSS subsystems and system components have been underway at NEON (see Metzger et al., 2014) and ICOS (see De Ligne et al., 2014). These studies indicate that substantial improvements to the IRGA system frequency response could be made by re-examining its GSS and components therein. The objective of this study is thus to produce an optimal combination of IRGA and GSS that (i) maximizes system practicability, and (ii) minimizes high-frequency spectral losses. In this endeavour, quantitative NEON requirements were used to evaluate the feasibility and degree to which these objectives were achieved. The overarching goal for such system is to permit unbiased, operational deployment and data processing across more comprehensive time and space domains for addressing the “Grand Challenges of Environmental Science”.

NEON selected an enclosed IRGA (LI-7200; LI-COR Biosciences, Lincoln, NE, USA) due to (i) instantaneous temperature and pressure compensation (Burba et al., 2012; Webb et al., 1980), (ii) improved frequency response compared to closed-path IRGAs (e.g., Burba et al., 2010; Fratini et al., 2012; Ibrom et al., 2007), and (iii) improved data coverage and lower maintenance compared to open-path IRGAs. We tested combinations of the LI-7200 and GSS components (intake tube, particulate filter, rain cap), both in the laboratory and in the field. Focused laboratory tests were performed to determine the general suitability of individual GSS components and their combinations. These tests addressed water ingress, pressure drop, as well as high-frequency spectral loss.

cal tube to the frequency attenuation by a membrane, and were conducted by different laboratories using varying equipment. Due to limited space in this study, only the key procedures are described below in a generalized form to provide the overall schemes and algorithms of testing. The results were aggregated to provide the range of performance across multiple tests.

2.1.1 Rain cap water ingress

In order to maximize data coverage and to minimize uncertainties in the latent heat flux determination, the GSS should be designed to minimize water ingress (NEON requirement NEON.TIS.4.1615). Different rain cap designs were tested for water ingress in a series of laboratory tests. Figure 1 shows three final rain cap designs; LI-COR's old rain cap (LO) until 2013, part number 9972-054, LI-COR's new rain cap (LN) from 2014, part number 9972-072, and the new NEON rain cap design (NN). Tests were conducted at a mass flow rate (standard temperature ($T = 20^\circ\text{C}$) and pressure ($p = 101.325\text{ kPa}$) conditions) of 23 SL min^{-1} (standard litres per minute) to emulate the worst case scenario. This significantly exceeded the minimal recommended volumetric flow rate (at temperature and pressure of measurement location) of 10.5 L min^{-1} (litres per minute) and nominal recommended volumetric flow rate of 15 L min^{-1} . The rain caps were sprayed from the top and side with a water hose at rates of $12.1\text{--}16.3\text{ L min}^{-1}$, including horizontal spray. Additional tests were conducted at 15 SL min^{-1} flow rate to establish whether a downward-oriented tube with 6.4 mm inner diameter (ID) would transport water upwards. Water ingress was observed, and the test concluded that a rain cap would indeed be required for the system to prevent or minimize water ingress. The latter corroborated the results reported for a downward-oriented tube without a rain cap from field tests conducted by ICOS (De Ligne et al., 2014).

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would be unity across all frequencies. In a real system, fluctuations in CO₂ or H₂O tend to be dampened at higher frequencies. Using power spectra to quantify transfer functions, the output variance or covariance is reduced to 50 % or –3 dB of its input at the half-power frequency $f_{50\%}$. Adding a rain cap, filter and intake tubing to an IRGA essentially acts as a low-pass filter. That is, it attenuates high-frequency fluctuations of H₂O and CO₂, which subsequently reduces the turbulent flux calculated via correlation with the vertical wind speed measurement. In order to allow automated procedures for high-frequency spectral corrections (e.g., Nordbo and Katul, 2012), the combined frequency response of the IRGA and its GSS shall be un-attenuated at frequencies ≤ 1 Hz (NEON requirement NEON.TIS.4.1626). Moreover, early results showed a wide range of frequency response for the particulate filters. Based on the above objective and Eqs. (7)–(10) below, we additionally specified that the filter shall have a half-power frequency $f_{50\%} \geq 4$ Hz (NEON requirement NEON.TIS.4.1627).

The transfer function of an IRGA system including the GSS can never be better than the spectral quality of the IRGA itself. Consequently, first the frequency response of the IRGA needs to be quantified. This allows subsequent determination of whether and for which GSS components optimization can warrant significant frequency response improvements. The LI-7200 optical unit measures CO₂ and H₂O number density at internal rates exceeding 100 Hz. In combination with minimal inertia thermocouples and pressure transducers for mole fraction conversion, LI-7200 frequency response is likely dominated by volume averaging in the optical cell with a volume of $V = 16.0 \text{ cm}^3$. The volume averaging effect can be quantified by the generalized transfer function of Silverman (1968), in the form of Massman (2004) and Moore (1986):

$$F_T(f) = \frac{\sin^2(\pi f \tau)}{(\pi f \tau)^2} \quad \text{with the time constant } \tau, \quad (1)$$

$$\tau = \frac{V}{Q_v}, \quad (2)$$

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π being number pi, and Q_v being volumetric flow rate. Analogously, Eq. (1) can be used to approximate the along-path (worst case) averaging effect of open-path gas analysers aligned to within $\approx 30^\circ$ of horizontal by determining τ as:

$$\tau = \frac{d_l}{U}, \quad (3)$$

with length of the optical path d_l (e.g., 12.5 cm for a LI-COR LI-7500) and horizontal wind speed U .

Subsequently, high-frequency attenuation was tested for the IRGA and each separate component of the GSS, as well as for cross-combinations of components, and for the complete system consisting of all listed components (Table 2). Two techniques were used for this purpose: (i) providing a CO_2 and H_2O change as a singular rising or falling step, and (ii) generating a square wave consisting of a sequence of many rising or falling steps. While (i) allows efficiently pre-screening a large number of parts, only (ii) provides the necessary sample size for determining stable results based on Fourier Transformation. The Fourier Transform of a perfect square waves' time derivative would show similar contributions across all frequencies, and the Fourier Transform of the actual time series' time derivative is the systems transfer function (Truax, 1999). In all experiments, solenoid switches were used to rapidly alternate between zero air and pre-defined concentrations of CO_2 and H_2O upstream of the tested component. The corresponding change was measured with a LI-7200 downstream of the tested component. In H_2O and CO_2 experiments the relative humidity (RH) and dry mole fraction varied between 0–90 % and 0–400 ppm, respectively. For H_2O specifically, the moist airstream was maintained at $\text{RH} > 90\%$ to reflect the field environment as well as possible. Nevertheless, for the square wave, the time-average over alternating dry and moist airstreams cannot exceed $\text{RH} = 50\%$. A dew point generator (for lower flow rates: LI-610, LI-COR Biosciences, Lincoln, NE, USA) or bubbler (for higher flow rates) in combination with a hygrometer (Optisure, Kahn Instruments, Wethersfield, CT, USA) were used to generate, control and record H_2O concentrations. Tests were performed for a minimum of 420 s, and LI-7200 variables were recorded at 50 Hz. In these tests,

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flow rates ranged from 9 to 35 SLPM depending on the experiment's goal, providing fully turbulent tube flow in the vast majority of tests (Reynolds number, $Re > 4000$) or upper range of transient flow in a few tests ($Re > 3300$).

Prior to the power spectra analysis (i) the first 200 s and last 20 s of data were discarded to focus on steady-state periods, (ii) missing values were linearly interpolated, (iii) the dry mole fraction time-derivative was calculated, (iv) the time-derivative was low-pass filtered with a 5th order Butterworth filter at 15 Hz half-power frequency to dampen leaking from high frequencies, (v) linear de-trending was applied to minimize bias, and (vi) 5% of the data at each end of the time series are tapered with a cosine-bell to reduce bias and to avoid leaking of peaks at far-away frequencies into other parts of the spectrum. Next, a fast Fourier transform was applied and unfolded spectral energy and co-spectra were calculated. A recursive circular filter with a Daniell kernel was then used to reduce noise, and the resulting Fourier coefficients were binned into exponentially widening frequency classes using the arithmetic mean. The result for the LI-7200 without additional GSS components $S_{\text{ref}}(f)$ corresponds to the reference transfer function of the LI-7200 in combination only with the experimental setup (solenoids, connectors, etc.). The results for the LI-7200 with additional GSS components $S_{\text{test}}(f)$ correspond to the test transfer functions of the LI-7200 in combination with the experimental setup as well as filter, intake tube and rain cap. Transfer functions $F_T(f)$ of filter, tube, rain cap as well as their combinations independent of LI-7200 and experimental setup were calculated by division of the individual power spectra (e.g., Foken et al., 2012). For this it is assumed that the mean spectral response between $f_1 = 0.01$ Hz and $f_2 = 0.2$ Hz was not attenuated:

$$F_T(f) = R_N \frac{S_{\text{test}}(f)}{S_{\text{ref}}(f)}, \quad \text{with the dimensionless normalization factor;} \quad (4)$$

$$R_N = \frac{\int_{f_1}^{f_2} S_{\text{test}}(f) df}{\int_{f_1}^{f_2} S_{\text{ref}}(f) df}. \quad (5)$$

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Noise was reduced by a circular filtering with a Daniell kernel. In cases where multiple test results were available, ensemble transfer functions and their ranges were calculated. Finally, $f_{50\%}$ was determined by inter/extrapolation of the resulting transfer function coefficients using the sigmoidal model of Eugster and Senn (1995):

$$F_T(f) = \frac{1}{1 + \left(\frac{f}{f_{50\%}}\right)^2}. \quad (6)$$

Resistor-capacitor theory then allows determining $f_{50\%}$ for a resulting system when multiple passive low-pass filters are combined, such as rain cap, filter and tube (e.g., Williams and Taylor, 2006):

$$f_{50\%} = 1.54 f'_{50\%} - 4.66 \text{ Hz, with the non-damped half-power frequency;} \quad (7)$$

$$f'_{50\%} = f_h \sqrt{2^{\frac{1}{n}} - 1}, \quad \text{the harmonic frequency;} \quad (8)$$

$$f_h = \frac{1}{2\pi \sqrt[n]{\prod_1^n \tau_n}}, \quad \text{and the time constant } \tau_n \text{ for each low-pass filter } n; \quad (9)$$

$$\tau_n = \frac{1}{2\pi f_{50\%,n}}. \quad (10)$$

The systems' damping coefficients in Eq. (7) were determined from an unweighted least-squares regression ($R^2 = 0.92$, p value = 6.338×10^{-8}): measured $f_{50\%}$ for several combinations of rain cap, filter and tube ($N = 14$) were regressed against $f'_{50\%}$ calculated from measured $f_{50\%}$ for individual components using Eqs. (8)–(10).

In addition to physical laboratory tests, high-frequency attenuation processes were also modelled using computational fluid dynamics (CFD) software (ANSYS, Canonsburg, PA, USA). To corroborate the experimental results, turbulent flow simulations of cases with well-mixed and plug-flow assumptions were performed. The CFD results

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consistently showed lower attenuation by the components than experimental data, indicating that a perfect step change or a perfect square wave is not achievable in real-life settings.

A variety of additional aspects need to be considered and warrant testing when optimizing an IRGA GSS. Of these, heating of the tube, filter and other components are addressed by the field experiments in this study (Sects. 2.2, 3.2), and by Fratini et al. (2012). Other tests are not the focus of this paper, such as optimization of tube length, tube material and flow rates, which have been covered both conceptually and experimentally by Burba et al. (2010); Clement et al. (2009); Fratini et al. (2012); Massman and Ibrom (2008); Rannik et al. (1997); Runkle et al. (2012).

2.2 Field tests

In July of 2013 and 2014 field tests were performed at the Niwot Ridge Subalpine Forest AmeriFlux US-NR1 site (see <http://ameriflux.ornl.gov/fullsiteinfo.php?sid=34>). The objectives of these tests were to determine (i) the impact and suitable dimensioning of intake tube heating, and (ii) whether the final GSS provides sufficient high-frequency response to warrant automated high-frequency spectral corrections in post-processing. To prevent condensation and to minimize attenuation of the water vapour measurement, the IRGA intake tube should be insulated and continuously heated with a constant wattage (NEON requirement NEON.TIS.4.2017). However, to enable mole fraction conversions to within manufacturer performance specifications, the temperature difference between IRGA inlet and outlet should be maintained to within $\leq 5^\circ\text{C}$ (NEON requirement NEON.TIS.4.1668). To ensure that IRGA drift with temperature remains within manufacturer performance specifications, the temperature difference between the IRGA block and inlet should be maintained to within $\leq 15^\circ\text{C}$ (NEON requirement NEON.TIS.4.1667). Lastly, to sufficiently improve H_2O frequency response for automated high-frequency spectral corrections, the heating wattage should be chosen so that relative humidity in the IRGA is maintained at $\leq 60\%$ (NEON requirement

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NEON.TIS.4.1666). Below this threshold, H₂O high-frequency attenuation behaves principally similar to CO₂ (e.g., Fratini et al., 2012).

2.2.1 Site description

US-NR1 is located in the Rocky Mountains, Colorado, USA (40°1'58" N, 105°32'47" W, 3050 m elevation), where measurements began in November 1998 (Monson et al., 2002; Turnipseed et al., 2002, 2003). The forest near the tower is around 110 years old, and primarily composed of subalpine fir (*Abies lasiocarpa* var. *bifolia*), lodgepole pine (*Pinus contorta*), and Englemann spruce (*Picea engelmannii*). The tree density is around 0.4 trees m⁻² with a leaf area index of 3.8–4.2 m² m⁻², tree heights of 12–13 m (Monson et al., 2010; Turnipseed et al., 2002) and an approximate displacement height of 7.8 m.

2.2.2 Instrumentation

All instrumentation used in the field tests was deployed on the US-NR1 tower at 21.5 m above ground, equivalent to 13.7 m above the displacement height. The companion study by Burns et al. (2014) provides an in-depth description of the sensor deployments, in short:

A Vaisala HMP35-D platinum resistance thermometer and capacitive hygrometer (Vaisala, Helsinki, Finland) was sampled at 1 Hz and was used in this study as reference for ambient air temperature (T_a) and relative humidity (RH_a).

A CSAT3 sonic anemometer (Campbell Scientific, Logan, UT, USA, S/N 0254, firmware v4) was used to measure the turbulent wind components. The measurements were performed in single-measurement mode at 10 Hz sampling rate, collected using the Campbell Scientific SDM protocol, and synchronized with variables from other sensors using network timing protocol (NTP). From the CSAT3, the along-axis, cross-axis and vertical-axis wind components as well as sensor health information (from the CSAT3 diagnostic word) were used in this study.

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from the LI-7200 through those from the LI-7500, and normalizing to the same spectral power between 0.005 and 0.05 Hz. The determination of the half-power frequency was then automated in the following way: (i) determining the frequency > 0.5 Hz for which the transfer function reaches its first minimum, (ii) recasting the transfer function Eq. (6) and solving for half-power frequency. Lastly, the spectral correction factors for the corresponding EC fluxes were determined by applying the transfer functions to the co-spectra of H₂O and CO₂ dry mole fraction and the vertical wind speed.

Before calculating the ensemble power spectra, all available periods were screened for (i) recorded maintenance activities and interruptions, and > 90 % raw data coverage (78 % half-hours remained), (ii) successful lag correction (70 % half-hours remained), (iii) undisturbed inflow sector (65 % half-hours remained), and (iv) measured variations in H₂O and CO₂ number density in excess of 5 : 1 signal-to-noise (instrument resolution) ratio (Lenschow and Sun, 2007, 46 % half-hours remained).

Lastly, in order to attribute the effect of intake tubes with different length d_l and inner diameter d_{id} , we solved the transfer function proposed by Philip (1963) in the form of Massman (1991) for half-power frequency:

$$f_{50\%} = \frac{\sqrt{\frac{-\ln(\sqrt{0.5})U^2}{\Lambda(\text{Re})d_l \frac{d_{id}}{2}}}}{2\pi} \quad (11)$$

with the longitudinal mean flow velocity in the tube U , and a linear interpolation of tabulated values (Table 1 in Massman, 1991) for the attenuation coefficient Λ (Re) (Lee and Gill, 1977, 1980).

3 Results and discussion

In the following, results for individual GSS components and their combinations are presented, based on laboratory tests (Sect. 3.1). Subsequently, the effect of different

heater settings and resulting frequency response for combined IRGA and GSS systems are shown, based on additional field tests (Sect. 3.2).

In order to determine the significance of GSS optimization, first of all the LI-7200 frequency responses were calculated. Numerically evaluating Eqs. (1) and (2) for Q_v leads to the simple linear relationship $Q_v = f_{50\%} \times 2.167 \text{ LPMHz}^{-1}$ ($R^2 = 1$; ρ value $< 2.2 \times 10^{-16}$). The minimum required volumetric flow rate to achieve the most stringent half-power frequency requirement of $f_{50\%} > 4 \text{ Hz}$ for the particulate filter can then be determined to be $> 8.7 \text{ Lmin}^{-1}$. Thus, at larger flow rates, the LI-7200 itself does not limit the objectives of the GSS optimization. For the flow rate set point of 10.8 SLmin^{-1} (corresponding to $\approx 13.6 \text{ Lmin}^{-1}$ and $\approx 16.2 \text{ Lmin}^{-1}$ under laboratory and site conditions, respectively), the LI-7200 operates at $f_{50\%} = 6.3 \text{ Hz}$ and $f_{50\%} = 7.5 \text{ Hz}$, respectively.

3.1 Laboratory tests

All high-frequency attenuation experiments suffered from the intrinsic inability to produce a perfect step change or a perfect square wave under real-life conditions. Response time of the laboratory setup (solenoids, effects of connectors and other physical mixing volumes upstream of a tested component) attenuate the step change itself. This resulted in an apparent reduction in frequency response of a tested component. A remedy was to normalize the results of the LI-7200 in combination with GSS components to the LI-7200 alone. Such procedure not only allowed the unveiling of the individual transfer functions of each GSS component, but also compensated for setup differences and enabled cross-comparison and aggregation of the results from the numerous different experiments. From our laboratory frequency response tests with the LI-7200 alone, we found $f_{50\%} = 3.4 \text{ Hz}$ for the combined effects of the LI-7200 and the laboratory setup. Using this together with $f_{50\%} = 6.3 \text{ Hz}$ for the LI-7200 itself in Eqs. (7)–(10) and solving numerically yields $f_{50\%} = 10.6 \text{ Hz}$ for the laboratory setup.

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3.1.1 Optimization of a rain cap

An important part of optimizing an enclosed IRGA EC system is determining which arrangement provides the best frequency response of the entire system. This would obviously be achieved by using a very short tube in the absence of any filter or rain cap.

5 However, for the practical reason to prevent precipitation from entering the filter and sampling cell, most experimental sites would benefit from using a rain cap. The rain cap is a mixing volume in interaction with the atmosphere, and a focus of our optimization is to determine which rain cap design provides the least frequency attenuation, while still preventing water ingress into the tube, filter and sampling cell.

10 Numerous rain cap designs have been tested conceptually using the CFD software to minimize sample mixing in the rain cap. Several designs have been selected, built and tested to limit water ingress in the laboratory experiments, and rain caps that ingested liquid water when sprayed horizontally while operating at 23 L min^{-1} flow were rejected. In addition, we found that adding a slight downward tilt to the intake tube
15 ($\approx 10^\circ$ from horizontal) helped avoid water ingress during the field tests (Sect. 3.2), which included periods of heavy precipitation. Consequently, the NEON requirement (NEON.TIS.4.1615) was fulfilled for the remaining designs, which were tested in the laboratory for frequency response following Eqs. (4) and (5). Figure 2 (top left panel) shows good frequency performance for LN and NN rain caps, with $f_{50\%} \geq 14.3 \text{ Hz}$ and
20 $f_{50\%} \geq 11.8 \text{ Hz}$, respectively (Table 3 provides an overview for all system components). Both newer rain caps considerably exceeded the performance of the older LO rain cap ($f_{50\%} \geq 2.4 \text{ Hz}$). However, both designs were still more limiting to high-frequency response compared to the filters with the best frequency response tested in Sect. 3.1.2.

25 ICOS conducted field tests of several additional rain caps for their LI-7200-based flux systems (De Ligne et al., 2014): (i) LI-COR's rain cap before 2013, part number 9972-043, which is a previous version of the LO rain cap, (ii) a modification of this rain cap with tubing extending all the way to the screen, (iii) a custom-built rain cap with lateral insertion and small volume were tested alongside (iv) a downward-oriented tube

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without a rain cap and (v) the LN rain cap. The range of results ($1.4 \leq f_{50\%} \leq 7.9$ Hz) was similar to our tests but slightly lower. Differences may be attributed to differing gas injection design in the laboratory, different experiment settings required for the field testing, and possible filter contamination. Their conclusion was that the frequency response of the LN rain cap assembly (6.4 ± 1.0 Hz) was second only to the downward-oriented tube, and the latter was found to provide insufficient water ingress protection. The experiments of De Ligne et al. (2014) also concluded that the rain cap critically contributes to overall system frequency response.

3.1.2 Optimization of a particulate filter

Similar to the rain cap situation, the highest frequency response of an enclosed IRGA EC system would be achieved without using a particulate filter. Such configurations are possible for a system based on the LI-7200 analyser, and have previously been used in the field (Burba et al., 2010, 2012; Clement et al., 2009). However, they would require frequent cleaning of the sampling cell in dusty environments or during high-contamination periods (e.g., harvest, pollination, etc.). To reduce the demand for cleaning, an intake particulate filter can be used. The important trade-off when optimizing the filter is to determine which models provide the least frequency attenuation with the smallest pressure drop, and still provide a pore size small enough to filter out most of the ambient particular contaminants. Figure 3 shows results from multiple laboratory experiments for such an optimization. Out of nine tested filters, the Swagelok FW-2.0 filter (Table 1 provides detailed filter specifications) had the lowest pressure drop (0.2 kPa at 10 SL min^{-1}), reasonably small high-frequency attenuation ($f_{50\%} \geq 14.9$ Hz), and still provided $2.0 \mu\text{m}$ particular filtering. The ZenPure PF-0.1 filter was a close second in pressure drop (0.6 kPa at 10 SL min^{-1}), but its frequency attenuation for CO_2 was much worse than the FW-2.0 at the high frequency range ($f_{50\%} \geq 8.3$ Hz), and its attenuation for H_2O was unacceptable ($f_{50\%} \geq 1.4$ Hz). Other tested filters had much larger pressure drops, which are not desirable for high-quality dry mole fraction computation, and which unnecessarily increase power consumption and wear on the system.

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ICOS conducted field tests of several additional filters for their LI-7200-based flux systems (De Ligne et al., 2014). A Pall open-face 2 μm filter (Pall Corporation, Port Washington, NY, USA) was tested for pressure drop alongside the FW-2.0 and AC-1.0. The AC-1.0 pressure drop was found unacceptable, and Pall 2 μm open-face filter was found to be less effective in contamination prevention as compared to the FW-2.0 filter. The pressure drop for the FW-2.0 filter in the De Ligne et al. (2014) experiments was small, on the order of 0.9 kPa for 10 L min⁻¹ at approximately sea level, but still 4–5 times the pressure drop found in our study. De Ligne et al. (2014) do not present half-power frequencies for individual GSS components, but state that addition of one of those filters did not significantly reduce LI-7200 system frequency response. The overall conclusion from both studies was similar suggesting the FW-2.0 filter to be optimal out of all tested models, and fulfilling the relevant NEON requirements (NEON.TIS.4.2007, NEON.TIS.4.1628, NEON.TIS.4.1618, NEON.TIS.4.1627).

3.1.3 Interaction of system components

Depending on the interaction of the system components reflected by Eq. (7), the total frequency response of the system may differ from a superposition of all components according to Eqs. (8)–(10). Hence, experiments were conducted to determine the actual effect of combining various system components on the total frequency response of the system, i.e. to parameterize Eq. (7). Figure 2 (top right and bottom panels) shows the results of such experiments for three main practical combinations of the components: (i) tube and filter, (ii) tube and rain cap, and (iii) combination of tube, filter and rain cap deployed together. Table 3 summarizes these and other results of laboratory experiments for various filters, rain caps, and their combinations.

Combining the tube and the FW-2.0 filter leads to a very minor effect on CO₂ frequency response as expected from the small volume of the filter and turbulent tube flow (11.9 Hz $\leq f_{50\%} \leq$ 15.4 Hz, Fig. 2 top right panel and Table 3). The H₂O response was noticeably affected, although to a relatively small degree (11.2 Hz $\leq f_{50\%} \leq$ 11.6 Hz). Such reduction in H₂O frequency response is expected because both filter and espe-

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cially the tube have large surface areas in relation to the sample volume and flow. The dipolar nature of the water molecule and surface adsorption/desorption rates proportional to relative humidity lead to a “sticky” behaviour of water vapour at the tube and filter surfaces. Such phenomenon was studied, modelled, and corrected for in a number of studies (e.g., Fratini et al., 2012; Massman and Ibrom, 2008; Rannik et al., 1997; Runkle et al., 2012). It can be partially remedied by heating the elements to reduce the relative humidity at the wall surface below 50–60 %. Below this threshold, H₂O behaves principally similar to CO₂ and theoretical corrections can be used to compensate for the frequency losses (Kaimal et al., 1972; Moncrieff et al., 1997). In the absence of heating, semi-empirical corrections progressive with relative humidity can also be used (e.g., Fratini et al., 2012; Massman and Ibrom, 2008; Runkle et al., 2012).

Combining the tube and rain cap led to a larger reduction in frequency response than combining the tube and filter for both CO₂ and H₂O ($2.0 \text{ Hz} \leq f_{50\%} \leq 12.0 \text{ Hz}$, Fig. 2 bottom left panel and Table 3). In fact, out of all elements in the system, the rain cap appeared to have the largest effect on the GSS frequency response. The importance of the rain cap choice was somewhat a surprise given that traditional closed-path GSSs utilize various custom-made rain caps with volumes exceeding several times those shown in Fig. 1. Yet, recent analyses by NEON (Metzger et al., 2014) and ICOS (De Ligne et al., 2014) corroborated the importance of the rain cap size and construction as a very sensitive component affecting EC system frequency response. The CFD simulations (data not shown) suggested that even small rain caps may experience vortices such that residence time of the sample in the rain cap exceeds that computed by simply dividing a rain cap volume by a flow rate (plug flow). This may explain why rain caps are responsible for a significant reduction in system frequency response in comparison to other components such as a short tube and a filter.

The frequency response of the combination of all elements in an enclosed IRGA EC system is shown in Fig. 2 (bottom right panel). The worst response was observed for the combination of the tube, FW-2.0 filter and the LO rain cap. This response was primarily driven by the effects of the rain cap (Fig. 2, top left panel) and yielded

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$f_{50\%} \geq 2.0$ Hz for the entire GSS for both CO_2 and H_2O (Table 3). Using the new, smaller rain caps significantly improved GSS system response, with half-power frequencies 2–6 times higher than with the LO rain cap. Differences among the GSS with the NN ($f_{50\%} \geq 9.3$ Hz) and LN ($f_{50\%} \geq 4.3$ Hz) rain caps were noticeable for both, CO_2 and H_2O , but overall both rain caps were much closer to each other compared to the LO rain cap. Also, these differences may be biased due to different sampling techniques, levels of relative humidity, and by how a step change or a square wave were generated in the laboratories. These tolerances were also apparent from a slightly better frequency response for the combination of tube, FW-2.0 filter and NL rain cap ($f_{50\%} = 12.0$ Hz) compared to the setup omitting the FW-2.0 filter ($f_{50\%} = 11.9$ Hz). Moreover, the laboratory tests of the NN rain cap did not include any dead volume potentially created by the rain caps' outer lip and leaking into the sample flow. While this lip adds rain protection and is vertically offset, it might increase air residence time in the vicinity of the rain cap, thus potentially providing a better response in the laboratory than might be attainable under field conditions.

Overall, we found that possible choices of filters ($f_{50\%} \geq 1.4$ Hz) and rain caps ($f_{50\%} \geq 1.9$ Hz) limit system frequency response compared to the LI-7200 sampling cell ($f_{50\%} \geq 6.3$ Hz) and a short and thin intake tube ($f_{50\%} \geq 15.9$ Hz). In order to better understand cross-sensitivity, we utilized Eqs. (7)–(10) and determined the frequency responses for all possible combinations of filters and rain caps, including those not explicitly tested (Fig. 4). It can be seen that for H_2O , the NN and LN rain caps provided similar frequency response, up to $\Delta f_{50\%} = 5$ Hz better compared to the LO rain cap. Yet, for NN and LN rain caps, the filter choice can decrease frequency response by as much as $\Delta f_{50\%} = -6$ Hz. For the LO rain cap, the effect of the filter choice was less pronounced, with a decrease in frequency response by as much as $\Delta f_{50\%} = -2$ Hz. It should be noted that for the two slowest filters AC-1.0 and PF-0.1, we determined $f_{50\%} < 0$, which is not physically feasible. However, the magnitude of underestimation falls within the standard error of regression Eq. (7). For CO_2 , the difference between NN and LN rain caps was slightly more pronounced compared to H_2O , with the NN rain cap

full effect of temperature fluctuations on density. So some of the fluctuations in density were large and well-resolved, but they did not actually contribute to the turbulent flux. In contrast, temperature-related density fluctuations are mostly attenuated in the LI-7200 cell (Burba et al., 2012).

Overall, no obvious improvement of H₂O frequency response was found for increasing heating power beyond 4 W. The resulting 8 °C temperature increase above ambient appeared to be sufficient, and the remaining field tests will focus on this heater setting, which is the only setting that also fulfils NEON's corresponding requirements (NEON.TIS.4.2017, NEON.TIS.4.1668, NEON.TIS.4.1667). Since the rain cap has been identified as a design priority in Sect. 3.1, we expected that decreasing the rain cap mixing volume would further improve frequency response for H₂O. However, for the 4 W heating setting, the LN rain cap did not appear to outperform the LO rain cap. This contradicts our laboratory findings, which suggest $f_{50\%} > 4$ Hz for the combination of LN rain cap with filter and tube. Also, during the LN rain cap period, filter and tube heating was actually 0.3 ± 0.9 W higher and RH_a was -13.1 ± 35.5 % lower compared to the corresponding LO rain cap period, which should have given the LN rain cap a slight advantage.

For the LN rain cap, CO₂ frequency response was found to be un-attenuated at frequencies ≤ 1 Hz under all RH conditions. A difference between the frequency response under heated and un-heated conditions appeared only for RH > 60 % and was not systematic (data not shown). The corresponding NEON requirement (NEON.TIS.4.1626) was thus fulfilled for CO₂.

In order to further investigate the impact of relative humidity on frequency response, we determined the half-power frequencies as described in Sect. 2.2.3 individually for each half-hour period. The results for the different GSSs and heating strategies are shown in Fig. 7 as a function of relative humidity. In general, 4 W of heating increased $f_{50\%}$ by 0.5–1 Hz. For RH_a < 40 %, the heated GSS with LN rain cap yielded $f_{50\%} > 3$ Hz, approaching the laboratory results of $f_{50\%} > 4$ Hz. At higher relative humidities,

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the heated GSS with LO rain cap outperformed the heated GSS with LN rain cap, contradicting our laboratory findings.

Together with the change from the LO to the LN rain cap, however, also the intake tube length was changed from 70 to 80 cm, and the ID from 4.8 to 5.3 mm. For the given flow rate set point of 10.8 SL min^{-1} (or $\approx 16.2 \text{ L min}^{-1}$ at site conditions), this lead to a reduction of the Reynolds number in the tube of -9.4% from $\text{Re} \approx 3470$ to $\text{Re} \approx 3150$. Following Eq. (11) the half-power frequency of the tube was thus reduced by -32.9% from 17.1 to 11.5 Hz. For the given volumetric flow rate, the LI-7200 cell by itself yielded $f_{50\%} = 7.5 \text{ Hz}$ due to volume averaging in Eq. (1). Combining LI-7200 cell and the tube according to Eqs. (7)–(10) yielded a half-power frequency reduction of -30.8% from 6.5 to 4.5 Hz due to the change in intake tube. This effect alone approximately offsets the gain in half-power frequency for changing from LO to LN rain cap as observed in the laboratory (Table 3, from 2.0 Hz to 4.3–6.1 Hz). In addition, not only did the tube inner volume increase by 42% from 12.4 to 17.7 cm^3 , but also the inner surface area increased by 28% from 104.5 to 133.2 cm^2 . As a result, the surface heating from the heater into the tube effectively decreased from $363.8 \pm 19.1 \text{ W m}^{-2}$ to $307.8 \pm 52.6 \text{ W m}^{-2}$. The combined effects resulting from changes in the tube ID and length increased the residence time in the tube, decreased turbulence in the tube, promoted surface adsorption of H_2O , and thus reduced the frequency response in particular under high relative humidity conditions. This explains that for a given 4 W heater setting, the GSS with LN rain cap performs similar to the GSS with LO rain cap for $\text{RH}_a < 60\%$, but performs worse for $\text{RH}_a > 60\%$. It should also be mentioned that the final NEON design uses a flow rate of 11.8 SL min^{-1} across sites, thus promoting turbulence development in the intake tube in excess of the setup studied here.

Applying Eqs. (7)–(10) to the half-power frequencies for the LI-7200 ($f_{50\%} = 7.5 \text{ Hz}$), 80 cm tube with 5.3 mm ID ($f_{50\%} = 11.5 \text{ Hz}$), filter FW-2.0 ($f_{50\%} = 17.4 \text{ Hz}$) and LN rain cap ($f_{50\%} = 12.05 \text{ Hz}$) yielded a system half-power frequency of $f_{50\%} = 3.1 \text{ Hz}$. This matched the field results in Fig. 7 at 35% relative humidity. Substituting in Eqs. (7)–(10) the 80 cm tube with 5.3 mm ID by the 70 cm tube with 4.8 mm ID ($f_{50\%} = 17.1 \text{ Hz}$), the

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was found to not limit frequency response. However, a 10 % increase in the tube length and inner diameter resulted in a 1/3 decrease in frequency response, effectively limiting the system. This was attributed to the reduction in surface heating and Reynolds number at given heater and flow rate settings, respectively. Heating the intake tube and particulate filter continuously with 4 W was found to improve the detectability of high-frequency H₂O fluctuations, and no further improvement was found for higher heating powers.

The National Ecological Observatory Network (NEON) has adopted a requirements-based approach for allowing its scientific infrastructure to address interactions of ecosystems, climate, and land use at pre-defined uncertainty levels. Here, this integrative strategy was applied to the development of an infrared gas analyser system for eddy-covariance applications. In this process, all but two of the corresponding technical requirements were fulfilled: (i) None of the tested heater settings were capable of continuously decreasing the relative humidity to $\leq 60\%$ in the gas analyser, and (ii) for high relative humidity levels the H₂O system response at 1 Hz was attenuated by up to 19 %. However, it was shown that the objective underlying these requirements can be accomplished, i.e. the application of adaptive correction procedures and automated data processing across field sites. This is a fundamental prerequisite for emergent environmental observatories such as NEON and the Integrated Carbon Observing System (ICOS): advancing ecological inference from local to continental scales rests on the shoulders of an integrated, unbiased, highly scalable and robust combination of instruments and data processing across eco-climatic zones.

Data availability

We provide an external supplement (see https://w3id.org/smetzger/Metzger-et-al_2015_IRGA-GSS) including (i) an extended abstract, (ii) a complete list of NEON requirements regarding dimensioning of the infrared gas analyser and its gas sampling system, (iii) a dimensional drawing of the NEON rain cap, as well as (iv) all NEON raw data used in this study accompanied by variable documentation.

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Table 1. Candidate filters and filter materials considered in this study, and their key characteristics including pore size (pore), length (d_l) and inner diameter (d_{id}).

Manufacturer	Filter model	Material	Pore [μm]	d_l [mm]	d_{id} [mm]	Abbreviation
3M/CUNO, Meriden, CT, USA	PolyPro XL G250 filter capsule	polypropylene housing and membrane	2.5	50.8	7.0	PP-2.5
3M/CUNO, Meriden, CT, USA	PolyPro XL G500 filter capsule	polypropylene housing and membrane	5.0	50.8	7.0	PP-5.0
Advantec MFS, Dublin, CA, USA	LS 25	stainless steel housing and nylon membrane	1.2	50.0	38.0	LS25-1.2
Advantec MFS, Dublin, CA, USA	LS 25	stainless steel housing and nylon membrane	5.0	50.0	38.0	LS25-5.0
Advantec MFS, Dublin, CA, USA	LS 47	stainless steel housing and nylon membrane	5.0	57.0	69.0	LS47-5.0
Pall Corporation, Port Washington, NY, USA	Acro 50	polypropylene housing and polytetrafluoroethylene (PTFE) membrane	1.0	82.0	73.0	AC-1.0
Swagelok, Solon, OH, USA	F-series	stainless steel housing and sintered stainless steel element	2.0	54.6	4.8	F-2.0
Swagelok, Solon, OH, USA	FW-series	stainless steel housing and pleated stainless steel mesh	2.0	54.6	4.8	FW-2.0
ZenPure, Manassas, VA, USA	PureFlo PTFE filter capsule	polypropylene housing and polytetrafluoroethylene (PTFE) membrane	0.1	127.0	73.0	PF-0.1

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Table 2. Components tested in detail in the laboratory and field experiments including LI-COR old (LO), LI-COR new (LN) and NEON new (NN) rain caps, and the Swagelok FW-2.0 filter (Table 1 provides detailed specifications). Key characteristics include length (d_l), inner diameter (d_{id}), outer diameter (d_{od}) and volume (V). Only components and materials selected for this study are shown, and numerous alternatives are excluded. Cross combinations were also tested.

Component	d_l [mm]	d_{id} [mm]	d_{od} [mm]	V [cm ³]
laboratory and field tests				
rain cap LO	17.5	36.0	41.9	17.8
rain cap LN	11.4	19.1	25.4	3.2
filter FW-2.0	54.6	4.8	25.4	1.0
sampling cell LI-7200	125.0	12.8	75.0	16.0
laboratory tests only				
rain cap NN	50.8	6.4–17.8	50.8	2.4
intake tube	700.0–1016.0	4.8–5.3	6.4	12.4–22.6
field tests only				
intake tube for rain cap LO	700.0	4.8	6.4	12.4
intake tube for rain cap LN	800.0	5.3	6.4	17.7

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Table 4. Descriptive statistics (median and median absolute deviation) covering periods of different heating settings of the LI-7200 intake tube and filter. The header distinguishes combinations of different rain caps (LO, LN) and heater settings (0 Watt, 4 Watt, 5 Watt, 6 Watt). Shown are ambient temperature (T_a), LI-7200 inlet temperature (T_{in}), LI-7200 outlet temperature (T_{out}), LI-7200 block temperature (T_{block}), ambient relative humidity (RH_a) and LI-7200 cell relative humidity (RH_{cell}).

Variable	LO-0 Watt	LO-4 Watt	LN-4 Watt	LO-5 Watt	LO-6 Watt
begin date	6 Jul 2013	2 Jul 2013	1 Jul 2014	11 Jul 2013	23 Jul 2013
end date	11 Jul 2013	6 Jul 2013	9 Jul 2014	23 Jul 2013	31 Jul 2013
heating power [W]	0.0 ± 0.0	3.8 ± 0.2	4.1 ± 0.7	5.4 ± 0.2	6.3 ± 0.1
T_a [°C]	15.1 ± 2.9	11.7 ± 3.0	12.8 ± 3.7	14.4 ± 3.2	11.8 ± 2.7
$T_{in} - T_a$ [°C]	0.2 ± 1.0	6.7 ± 0.7	7.7 ± 1.6	9.6 ± 0.9	12.7 ± 1.0
$T_{in} - T_{out}$ [°C]	-0.1 ± 0.2	3.7 ± 0.2	4.0 ± 0.9	5.5 ± 0.3	6.9 ± 0.2
$T_{in} - T_{block}$ [°C]	-0.3 ± 0.2	5.7 ± 0.3	6.0 ± 1.4	8.4 ± 0.5	10.6 ± 0.4
RH_a [%]	46.1 ± 10.8	63.1 ± 14.6	50.0 ± 20.9	55.5 ± 29.6	68.7 ± 17.8
RH_{cell} [%]	44.7 ± 12.2	48.7 ± 13.7	39.0 ± 15.2	38.5 ± 20.9	41.7 ± 11.3
$RH_a - RH_{cell}$ [%]	1.0 ± 2.9	14.9 ± 1.9	11.6 ± 4.8	16.2 ± 8.2	24.7 ± 7.2
sample size (half-hours)	190	183	284	288	275

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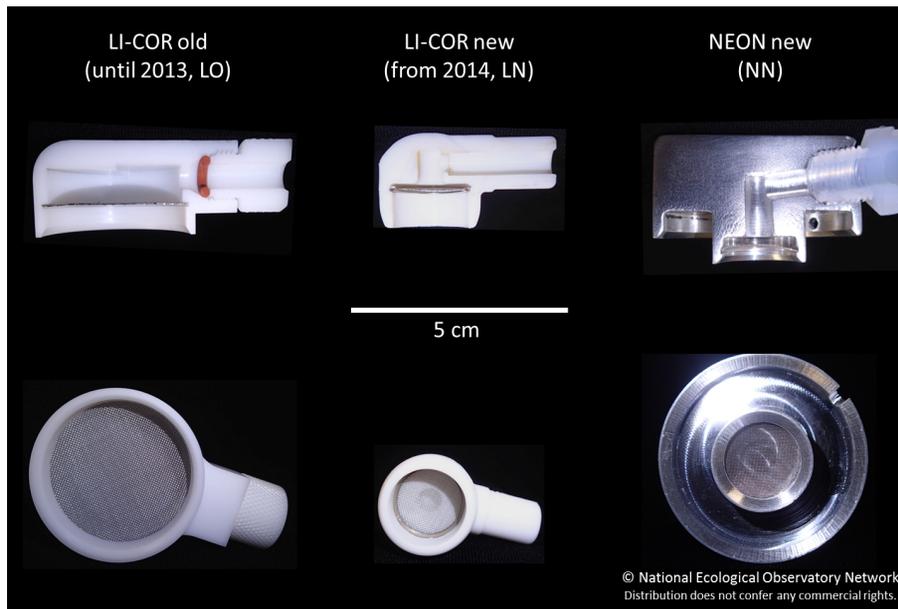


Figure 1. Three selected rain cap designs tested in this study. Top row: cross-sections of each rain cap showing their internal volumes. Bottom row: rain cap inlets with screens that face downwards in typical field deployments.

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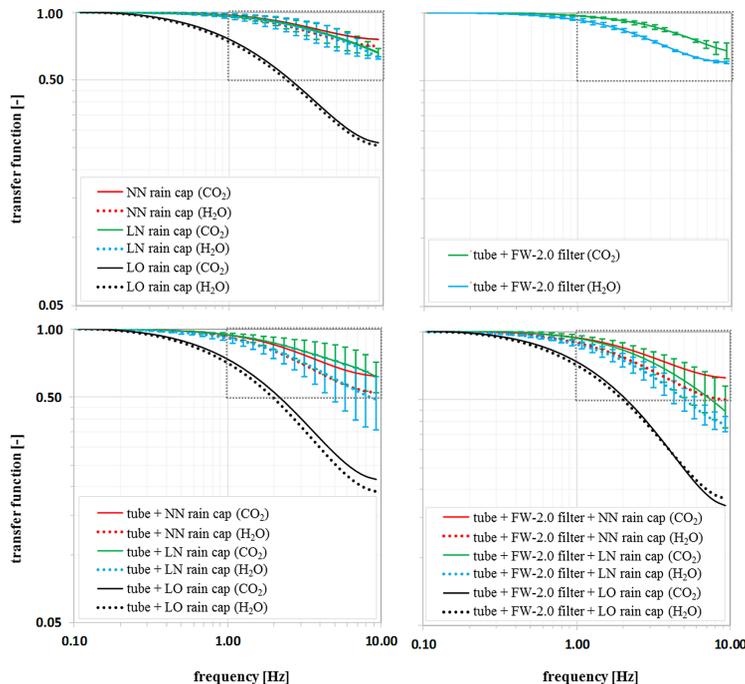


Figure 2. Transfer functions of different gas sampling system components and combinations thereof, without heating or insulation. Dotted grey boxes indicate approximate desirable ranges for a short-tube low-power implementation, requiring minimal corrections. Bars indicate range from multiple experiments, where available, as described in Sect. 2.1. Please note that the y axis starts at 0.05. Top left panel: three selected rain caps NEON new (NN), LI-COR new (LN) and LI-COR old (LO), without tube and filter. Top right panel: tube and Swagelok FW-2.0 filter (Table 1 provides detailed specifications), without rain cap. Bottom left panel: tube and three selected rain caps, without filter. Bottom right panel: tube, FW-2.0 filter and three selected rain caps.

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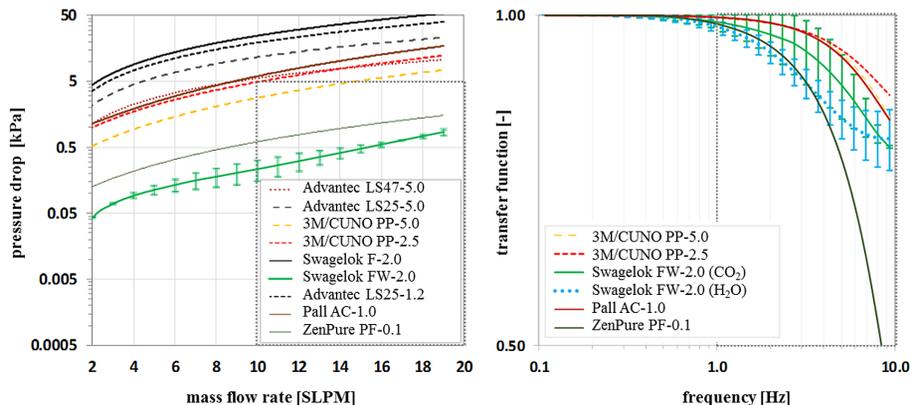


Figure 3. Optimization of an intake particulate filter. Dotted grey boxes indicate approximate desirable ranges for a short-tube low-power implementation, requiring minimal corrections. Left panel: pressure drop of nine tested filters at different flow rates, without tube and rain cap (Table 1 provides detailed filter specifications). Please note the log-scale of y axis. Right panel: transfer function of five selected filters, without tube, rain cap, heating or insulation. Please note that y axis starts at 0.5. Bars indicate range from multiple experiments, where available, as described in Sect. 2.1.

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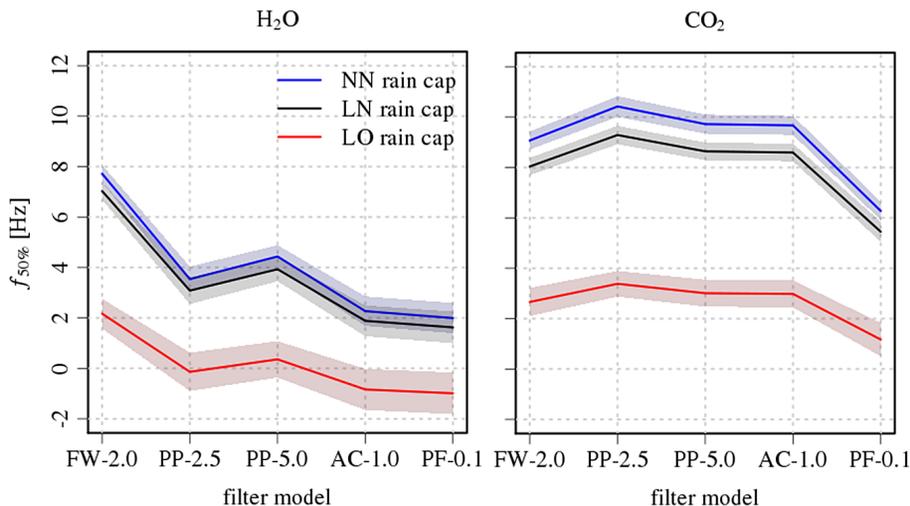


Figure 4. Half-power frequencies of filter and rain cap combinations without tube for H₂O (left panel) and CO₂ (right panel). Rain caps are NEON new (NN), LI-COR new (LN) and LI-COR old (LO). Filters are Swagelok FW-2.0, 3M/CUNO PP-2.5, 3M/CUNO PP-5.0, Pall AC-1.0 and ZenPure PF-0.1 (Table 1 provides detailed filter specifications). Values are determined by propagating combinations of individual filter and rain cap half-power frequencies (Table 3) through Eqs. (7)–(10). The shaded areas represent the standard error resulting from regression Eq. (7).

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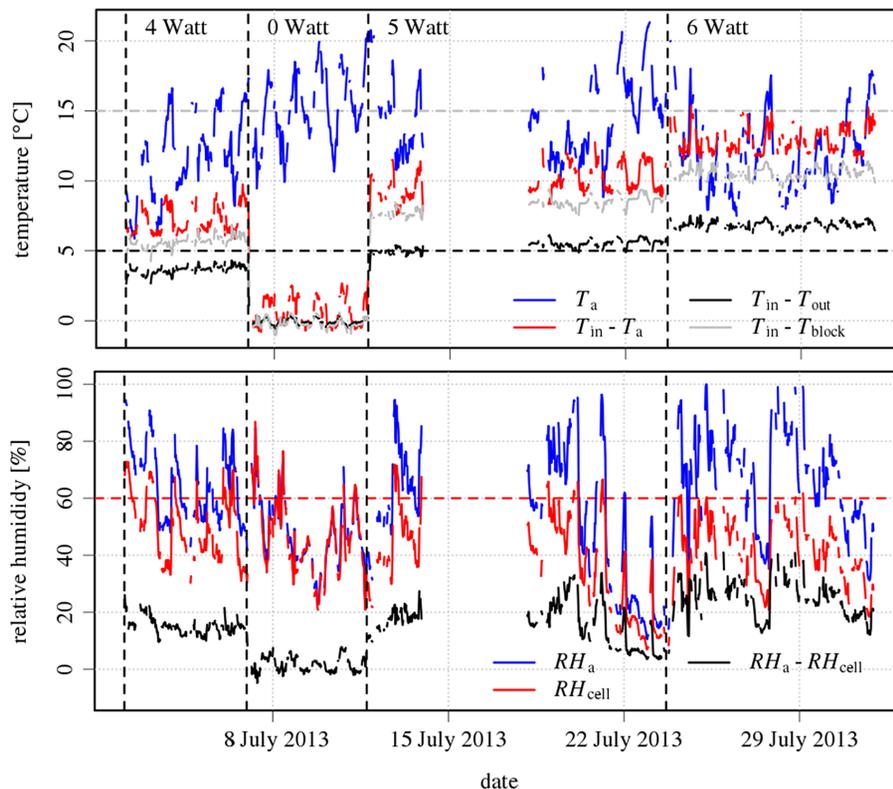


Figure 5. Example time series of the ambient air temperature and relative humidity during periods of different heating settings of the LI-7200 intake tube and filter, indicated by the dashed vertical lines. Top panel: ambient air temperature (T_a), LI-7200 cell inlet, outlet and block temperature (T_{in} , T_{out} , T_{block} , respectively) and differences thereof. The dashed horizontal line indicates a 5°C threshold for the temperature gradient across the LI-7200 cell. Bottom panel: ambient relative humidity (RH_a), in the LI-7200 cell (RH_{cell}), and differences thereof.

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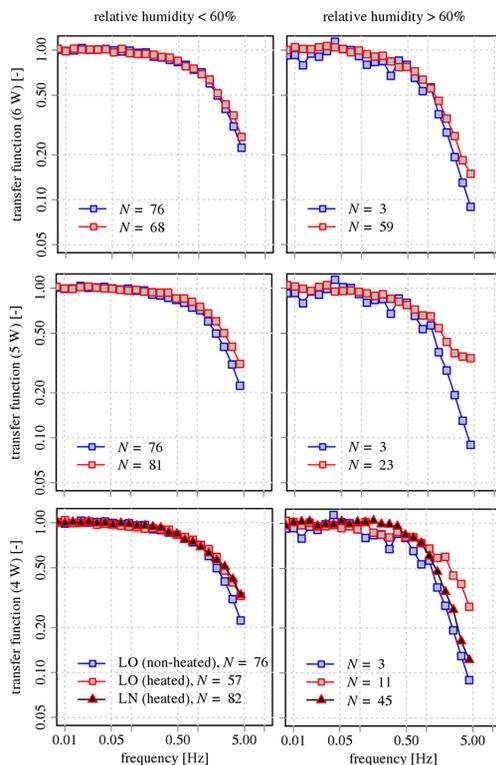


Figure 6. Ensemble transfer functions of LI-7200-measured H_2O number density relative to LI-7500 for different heater settings of the intake tube and filter (rows) and ambient relative humidity classes (columns). Shown are results for the LI-COR old (LO) rain cap with and without heating of filter and intake tube, as well as for the LI-COR new (LN) rain cap for the 4 W heater setting, together with the respective ensemble sample size (N). Only half-hours with sensible heat flux $> 50 \text{ W m}^{-2}$ are used to homogenize the sample size across different test periods.

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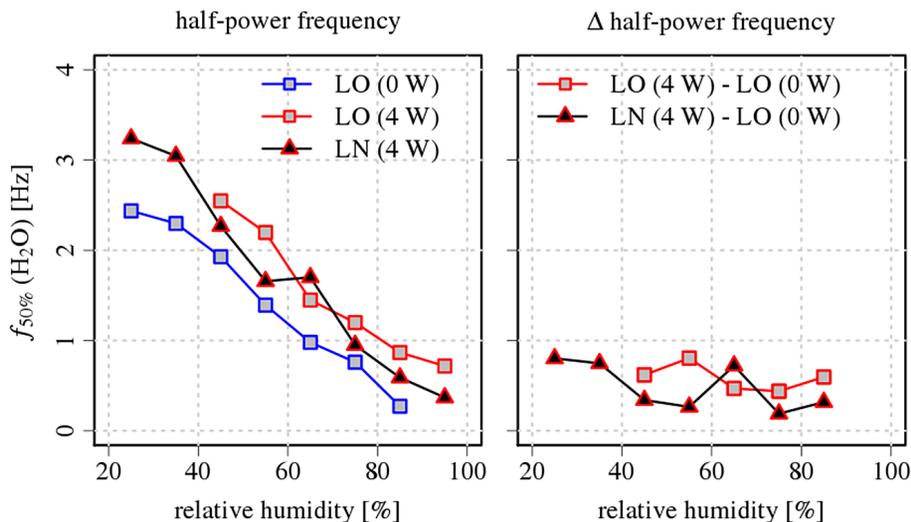


Figure 7. Ensemble half-power frequencies of LI-7200-measured H_2O number density relative to LI-7500 as function of ambient relative humidity. Relative humidity classes without ensemble member are omitted. Left panel: results for the LI-COR old (LO) rain cap without heating of filter and intake tube, as well as the LO and LI-COR new (LN) rain caps for the 4 W heater setting. Right panel: differences in half-power frequency between LO and LN rain caps with 4 W heating of filter and intake tube, and the LO rain cap without heating of filter and intake tube.

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