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EddyUH: an advanced software package for eddy covariance flux calculation for a wide range of instrumentation and ecosystems

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Abstract

We have carried out an inter-comparison between EddyUH and EddyPro®, two public software packages for post-field processing of eddy covariance data. Datasets including carbon dioxide, methane and water vapour fluxes measured over two months at a wetland in Southern Finland and carbon dioxide and water vapour fluxes measured over three months at an urban site in Helsinki, were processed and analysed. The purpose was to estimate the flux uncertainty due to the use of different software packages and to evaluate the most critical processing steps, determining the largest deviations in the calculated fluxes. Turbulent fluxes calculated with a reference combination of processing steps were in good agreement, the systematic difference between the two software packages being up to 2% and 6.7% for half-hour and cumulative sum values, respectively. The raw data preparation and processing steps were consistent between the software packages, and most of the deviations in the estimated fluxes were due to the flux corrections. Among the different calculation procedures analysed, the spectral correction had biggest impact for closed-path latent heat fluxes, reaching nocturnal median value of 15% at the wetland site. We found up to 43% median value of deviation (with respect to the run with all corrections included) if closed path carbon dioxide flux is calculated without the dilution correction, while the methane fluxes were up to 10% lower without both dilution and spectroscopic corrections. The density (and spectroscopic) correction was the most critical step for open-path systems. However, we found also large spectral correction factors for the open-path methane fluxes, due to the sensor separation effect.

1. Introduction

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The eddy covariance (EC) technique is the most direct and defensible way to measure and calculate vertical turbulent fluxes of momentum, energy and gases between the atmosphere and biosphere. During the last three decades, the number of long-term EC stations all over the world has increased exponentially covering a wide range of different ecosystem types (FLUXNET, www.fluxdata.org). EC is a technique analyzing high-frequency wind and scalar atmospheric data series (often called "raw data") usually saved in hard drive devices for post-field processing and final estimations of turbulent flux values. During the past years several attempts have been made to standardize the processing methodology at least for carbon dioxide (CO_2), sensible and latent heat (LE) fluxes (Aubinet et al., 2000; Aubinet et al., 2012; Lee et al., 2004). However, the harmonization of data processing is quite difficult, since most of the required steps and corrections are site and instrument (gas analyzer and sonic anemometer) specific. Nowadays, new and better instrumentation is available for measuring turbulent fluxes of energy and matter using the EC technique. Recent studies have compared commercially available gas analysers focusing on precision, stability and systematic and random errors both for CO_2 fluxes (Burba et al., 2008; Ibrom et al., 2007a; Järvi et al., 2009), and methane (CH_4) and nitrous oxide (N_2O) fluxes (Detto et al., 2011; Peltola et al., 2014; Peltola et al., 2013; Rannik et al., 2015). However, only a few studies have reported an inter-comparison between EC software packages, and all focusing only on energy and CO_2 fluxes (Fratini and Mauder, 2014; Mauder et al., 2008; Mauder et al., 2007). For example, Mauder et al. (2008) concluded that the data preparation, the coordinate rotation of sonic anemometer wind components and the different approaches for high frequency spectral correction are critical processing steps, giving differences up to 10% in their exercise. Fratini and Mauder (2014) compared TK3 and EddyPro® software packages, achieving a satisfying agreement in calculated fluxes and related quality flags only after tuning the software processing steps and corrections to be similar. In fact, systematic differences in EC flux estimates strongly depend on the selection, application and order of processing steps, and the correct application, order and sometimes relevance and consequences of several processing steps are still topics under discussion (Aubinet et al., 2012; Mauder and Foken, 2006). In addition, the relevance of some processing steps and corrections depends not only on the system setup, but also on meteorological conditions and ecosystem types (e.g. Mammarella et al. (2015); Nordbo et al. (2012)). As a result, the EC processing softwares available to the community feature different implementations: some steps may be implemented using different methods (Mauder et al., 2007), while some operations and eventually further corrections suggested by recent findings are not supported by some of the softwares. This is particularly relevant for gases like CH_4 and N_2O for which the deployment of the EC system with easy-to-use fast response analysers have become popular only during the last decade. Therefore, neither data processing approaches have yet been standardized nor software inter-comparison studies have been published for these gas fluxes.

In this study, we have performed an inter-comparison between EddyUH and EddyPro, two public and commonly used software packages for EC data processing and calculation. The aims are to estimate the flux uncertainty due to the use of different software packages at half-hour as well as for cumulative sums, and to assess the most critical processing steps, determining the largest deviations in the calculated fluxes. We focus not only on LE and CO_2 fluxes, as it has been done in previous studies, but also on CH_4 fluxes.

2. Material and methods

2.1 Software description

EddyUH is a software package for EC raw data processing, developed by the Micrometeorology Group at the Department of Physics, University of Helsinki (Finland). EddyUH, which is freely downloadable from https://www.atm.helsinki.fi/Eddy_Covariance/EddyUHsoftware.php, is written in Matlab and includes a graphical user interface (GUI). In order to advance methodological issues (concerning especially CH_4 and N_2O fluxes), besides standardized procedures, the most recent corrections and methods have been also implemented in EddyUH (see Table 1).

Post-field EC data processing with EddyUH is done through user-defined projects. A project in this context means a certain time period of data from a certain site which are processed with certain user-defined processing methods. These methods are determined by the user using the GUI and are saved in a setup-file where also the site specifics and measurement system characteristics among other things are defined. Therefore, all the processed data are always related to the saved project. The same project may include up to five different gas analysers combined with the same ultra-sonic anemometer, giving the possibility for the user to process several raw data sets at the same time. The software includes a number of modules, which operate at different levels of post-processing (Fig.1). Preliminary fluxes are calculated in the pre-processor, where the first level of processing is done to the raw dataset. Then several corrections are applied in the flux-calculation module, and the final fluxes are calculated (Table 1). In order to optimize the processing and properly apply all needed corrections, several software tools are available (Fig. 1). Co-spectral data are used in the high frequency spectral transfer function estimator, where the low pass filter time constant is experimentally estimated for each gas according to Mammarella et al. (2009). This approach is particularly relevant in case of closed-path systems. Further, the time lag optimizer is an useful tool to verify the correctness of the chosen time lag window (and eventually refine it) for each gas, as well as to determine the varying window boundaries for H_2O as explained in Appendix A. Finally, other modules are available in EddyUH, for example for analyzing the estimated spectra and co-spectra, for calculation of flux uncertainties, and for determining the flux footprint statistics according to the Kormann and Meixner (2001) model (Fig. 1).

The EddyUH software was compared against EddyPro, perhaps the most used software in the EC flux community, developed by LI-COR Biosciences Inc. (Lincoln, NE, USA). It is freely available and well documented (www.licor.com/eddypro). The results presented in this study are based on EddyUH version 1.7 and EddyPro version 5.2.1.

2.2 Site description and measurements

The software inter-comparison was performed using datasets from two field sites in Southern Finland. The first dataset was collected at Siikaneva fen site (61˚49.961' N, 24˚11.567' E) during the CH_4 inter-comparison field campaign (Peltola et al. 2013). The EC data used in this study were measured during 1.5. – 30.6.2010 with a 3D sonic anemometer (USA-1, Metek GmbH), two closed-path (LI-7000, LI-COR Biosciences; G1301-f, Picarro Inc.) and one open-path gas analyser (LI-7700, LI-COR Biosciences). LI-7700 was an early prototype version of the later commercialised LI-7700. LI-7000 measured CO_2 and H_2O and G1301-f measured CH_4 and H_2O molar fractions, whereas LI-7700 measured CH_4 molar densities. LI-7000 and G1301-f used a shared heated sampling line that was approximately 16.8 m long (ID: 10 mm, flow rate: 24 LPM). The sonic anemometer was situated 2.75 m above peat surface and the open-path LI-7700 directly below it, causing a 45 cm vertical separation between the sensors. Further details about the site and measurements can be found from Peltola et al. (2013).

The second dataset was collected between 1.7. – 30.9.2010 at the Erottaja site located in the Helsinki city centre (60˚09.912' N, 24˚56.723' E). The measurements represent densely built up urban area with only 5% of the surface being covered with vegetation. The measurements are carried out in a 3.8 meters high mast located on top of a 38 meters high fire station tower resulting in a total height of 41.8 meters. This is a sufficient height for the EC measurements as the mean building height in the surroundings of the tower is 21.7 meters. The measurement setup consisted of an ultrasonic anemometer (USA-1, Metek GmbH) to measure the wind components and an open- and enclosed-path infrared gas analysers (LI-7500 and LI-7200, LI-COR Biosciences) for the CO_2 and water vapour (H_2O) fluctuations. Details of the measurement setup can be found in Nordbo et al. (2013).

2.3 Turbulent flux calculation

The turbulent fluxes of CO_2 (F_{CO2}, µmol m^{-2}s^{-1}), CH_4 (F_{CH4}, nmol m^{-2}s^{-1}), sensible (H, W m^{-2}) and latent (LE, W m^{-2}) heat are calculated from the covariances between a respective scalar and vertical wind velocity (w) as:

$$F_{CO2} = \frac{\rho_d}{M_a}\overline{w'\chi_{CO2}'}, \quad (1)$$

$$F_{CH4} = \frac{\rho_d}{M_a}\overline{w'\chi_{CH4}'}, \quad (2)$$

$$H = \rho_d c_p \overline{w'T'}, \quad (3)$$

$$LE = \rho_d L_v \frac{M_w}{M_a}\overline{w'\chi_{H2O}'}, \quad (4)$$

where ρ_d is the dry air density (kg m^{-3}), c_p the specific heat capacity of dry air (J kg^{-1} K^{-1}), L_v is the latent heat of vaporization for water (J kg^{-1}), T the temperature (K) and M_a and M_w the molar masses of dry air and water, respectively. The terms $\overline{w'T'}$, $\overline{w'\chi_{CO2}'}$, $\overline{w'\chi_{CH4}'}$ and $\overline{w'\chi_{H2O}'}$ are the covariances between w and T, dry mole fractions of CO_2, CH_4 and H_2O, respectively. Overbars and primes represent temporal averaging and fluctuations, respectively. A brief description of post-field data processing operations and methods, as presented in Table 1, are given in Appendices A and B.

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
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Atmospheric Measurement Techniques Discussions

2.4 Setup of software runs

Both datasets were processed using the reference combination of processing steps (Fig. 2) and available methods implemented in EddyUH and EddyPro (Table 2). The applied methods were the same for most of the steps. However, some differences between softwares were present. In EddyUH the rawdata despiking was done by the difference limit method (Appendix A), while in EddyPro the Vickers and Mahrt (1997) method was used. Different experimental methods were applied for spectral correction, e.g. according to Mammarella et al. (2009) in EddyUH and Fratini et al. (2012) in EddyPro. Moreover, additional correction for absorption line pressure broadening caused by H_2O to closed-path CH_4 was done in EddyUH according to Rella (2010). The same correction is not implemented in EddyPro. Finally, we performed four different combinations of processing steps and compared them with the reference combination in order to evaluate the effects of different calculation steps on the final flux estimates. The alternative runs were setup by modifying one step of the reference combination at a time. The first and second runs were done excluding the spectral correction and applying the theoretical approach (instead of experimental one used in the reference combination), respectively. The density and spectroscopic corrections were omitted in the third run, and finally in the final run a constant value for the time lag was used.

Flux data was quality screened prior to analysis. CH_4 flux data was removed if the CH_4 mean mole fraction was above 5 or below 1.7 ppm. Additionally, LI-7700 fluxes were discarded if the received signal strength indicator (RSSI) was below 15. All the Siikaneva flux data were discarded if the second coordinate rotation angle (used to set $\overline{w}=0$) was above 10°. Wind direction (90-180° omitted) was used to omit periods when the measurement system at the Erottaja site was in the wake of the building. Also, periods when there were known problems with the measurement setup at the Erottaja site were discarded. Plausibility limits were also used, since if the flux values were outside certain predefined limits they were thought to be unphysical. For Siikaneva data these limits were -50 and 160 nmol m^{-2} s^{-1} for F_{CH4}, -30 and 600 for LE and -20 and 20 for F_{CO2}. For Erottaja data following limits were used: -30 and 500 for LE and -10 and 60 for F_{CO2}. Finally, flux data were discarded if the corresponding quality flags, as determined by EddyUH and EddyPro, were above 5 based on the Foken et al. (2004) flagging policy. The data coverage obtained after data screening is given in Table 3.

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Published: 18 January 2016

Atmospheric Measurement Techniques Discussions

3. Results

3.1 Flux comparison between software packages

Fluxes measured by the same system were analysed and compared as estimated by the two software packages in the reference run. In terms of regression statistics, the best agreement between EddyUH and EddyPro was obtained for LE and F_{CO2}, and LE and F_{CH4} measured by closed-path systems LI-7000 and G1301-f, respectively, at Siikaneva (Figs. 3d,e and 3c,a) and F_{CO2} by LI-7200 at Erottaja (Fig. 3i). For LI-7500 LE and F_{CO2} no systematic differences between the software packages were found (Figs. 3f and 3h) even though the data show more scatter around the 1:1 line (r^2=0.91, rmse=1.29 W m^{-2} for LE and r^2=0.98, rmse=0.12 μmol m^{-2} s^{-1} for F_{CO2}) than the other analysers. The scatter was caused by spurious values for spectral corrections (attenuation factor occasionally below 0.7 in EddyPro) and the scatter was removed if the periods with unrealistic spectral corrections were removed (figure not shown). Instead, a systematic difference was found for LE measured by the LI-7200 analyser in Erottaja, being the EddyPro fluxes 2% higher than those calculated by EddyUH (Fig. 3g).

Finally, good agreement resulted from the LI-7700 F_{CH4}, being the slope equal to unity (r^2=0.98 and rmse = 0.88 nmol m^{-2} s^{-1}, Fig. 3b). However, the sensor separation correction in EddyPro (Horst and Lenschow, 2009) caused relatively large scatter between LI-7700 fluxes and if the correction was omitted, visually the scatter between the two software packages was reduced, although regression statistics were slightly worse (y = 0.94x+0.51, rmse = 1.21 nmol m^{-2} s^{-1}, r^2=0.99) (figure not shown). Applicability of the sensor separation correction for this particular dataset is discussed in Sect. 4.2.

In order to further evaluate the discrepancies between the two software, diel patterns of flux ratio (left side in Fig. 4) and bias (right side in Fig. 4) were plotted for each flux at different processing levels. In general, the uncorrected (raw) fluxes do not show significant deviations from unity (left side of Fig. 4) or from the zero line (right side of Fig. 4), which suggest that the preparations done at the raw data level (despiking, coordinate rotation, time lag compensation) did not cause significant systematic differences to the fluxes. For LE calculated from LI-7500 data, the WPL correction tends to be slightly larger in EddyUH than in EddyPro, meaning that it increases more the daytime positive fluxes (cf. WPL curve in Fig. 4r). The daytime WPL correction in EddyUH is approximately 2 W m^{-2} larger than in EddyPro, which corresponds to daytime relative difference of 4% (Fig. 4q). For closed-path analysers or other open-path fluxes there is no difference in the WPL correction and the uncorrected and WPL corrected curves follow similar pattern. The biggest differences between the software's were related to the spectral corrections. For closed-path LI-7000 and G1301-f the fully corrected (e.g. WPL+SC in Fig. 4) LE fluxes were approximately 7% larger at night-time in EddyUH than in EddyPro (Figs. 4m and 4k). However, during these periods the absolute difference was still below 1 W m^{-2}, since the night-time LE are small. This difference is due to different RH dependence of low pass filter time constant found between the two software's (see discussion in Sect. 4.1). For LI-7700 F_{CH4} the relative difference between the software packages was on average 12% during night, EddyPro fluxes being larger (Fig. 4c), which corresponds to absolute difference of 1-4 nmol m^{-2} s^{-1} (Fig. 4d). This difference was related to the sensor separation correction and the difference was smaller (4-10 % or 0.5-1.5 nmol m^{-2} s^{-1}, EddyUH fluxes were larger) if the correction was not done in EddyPro (see the corresponding discussion in Sect. 4.2).

3.2 Flux comparison between instruments

Fluxes measured with different gas analysers are compared as estimated using the reference combination in EddyUH and EddyPro (Fig. 5). At Erottaja, very good agreement was found between F_{CO2} measured by LI-7200 and LI-7500 (Figs. 5e and 5f) and similar results were obtained by using EddyUH (slope = 0.99, r^2 = 0.92, rmse=1.25 μmol m^{-2} s^{-1}) and EddyPro (slope = 0.98, r^2 = 0.90, rmse =1.32 μmol m^{-2} s^{-1}). LE measured by the same gas analysers show slightly weaker correspondence, the slope and rmse being 1.02 and 8.15 W m^{-2} for EddyUH and 1.06 and 8.36 W m^{-2} for the EddyPro run, respectively (Figs 5g, and 5h). The small difference in LE between the two software is likely due to the spectral corrections (see below). Overall, the results are in agreement with Nordbo et al. (2013), who also found a better agreement between F_{CO2} than LE measurements at the same site. A very good correspondence (slope=0.97; r^2=1.00, rmse = 1.94 W m^{-2}) was found between LE measured by LI-7000 and G1301 systems for the EddyUH reference run at the Siikaneva site (Fig.5c). For EddyPro similar statistics were obtained (slope=0.96, r^2=1.00, rmse = 2.56 W m^{-2} in Fig.5d). By using the reference combination in EddyUH run, a relative good agreement was also obtained between F_{CH4} measured by G1301 and LI-7700 (Fig. 5a). The regression statistics (slope=1.09, r^2=0.84, rmse=2.64 nmol m^{-2} s^{-1}) are similar to the ones reported in Peltola et al. (2013). A 16% difference between the two F_{CH4} was found in the EddyPro run (Fig. 5b), because of larger spectral correction estimates for the open-path gas analyser(see Sect. 4.2).

3.3 Effects of different flux processing combinations

The impact of calculation steps on the final flux estimates in EddyUH and EddyPro is presented as deviation (in %) from the reference run for Siikaneva (Fig. 6) and Erottaja (Fig.7) datasets. For closed-path systems in Siikaneva, the run without spectral correction had the largest effect on LE, being (in the EddyUH run) 14% and 9% lower for G1301-f, and 16% and 12% lower for the LI-7000 system, during night- and day-time, respectively (Fig.6c and 6d). When compared to EddyUH run, slightly smaller deviations (10% and 8% for G1301-f and 12% and 11% for the LI-7000) were found in the EddyPro run, but the trend in the deviations were consistent between the softwares. Similar range of deviations was found in Erottaja LE measured by LI-7200 (Fig.7b). However, performing the theoretical spectral correction to the Siikaneva LE had a minimal effect (Fig. 6c and 6d), while the deviations found in LE measured by LI-7200 at Erottaja ranged between 6 and 3% (Fig.7b). The use of a constant time lag produces a small effect on LE, except during night-time when the higher relative humidity increases the sorption of H_2O in the sampling line walls (Nordbo et al., 2014) and H_2O time lag becomes larger than its nominal value. At Siikaneva the theoretical spectral correction produces up to 7% higher F_{CO2} and F_{CH4} measured by LI-7000 and G1301-f systems, respectively, respect to the experimental spectral correction (used in the reference run). If the LI-7000 F_{CO2} is calculated without performing the dilution correction (e.g. using the wet mole fraction), we obtained 43% higher daytime CO_2 uptake with both softwares, and about 3% lower positive fluxes during night-time. The same correction has also relevant impact on daytime F_{CH4} measured by G1301-f, resulting in 10% and 6% deviations in EddyUH and EddyPro, respectively.

For open-path systems the critical step is represented by the density (and spectroscopic) correction. In Erottaja, the net CO_2 emission calculated from LI-7500 data without density correction is underestimated by 38% and 37% during daytime in EddyUH and EddyPro, respectively (Fig. 7c). Instead, the nocturnal F_{CO2} is 8% smaller than from the reference run. Although the effect of no WPL is lower on LE, the calculated deviations are still relevant, being 15% and 12% during day time (in EddyUH and EddyPro, respectively), and 4 % and 3% during night-time. Finally, in Siikaneva the LI-7700 F_{CH4} calculated in EddyUH without density and spectroscopic correction shows -71% and 20% deviations from the reference run during day and

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night time. The same median values estimated in EddyPro are -67% and 18% (Fig. 6b). In addition, it can be seen from the same figure that the deviation of nocturnal F_{CH4} calculated without spectral correction (no spec run) in EddyPro is larger (-21%) than the one obtained in EddyUH (-8%). This is consistent with the fact that EddyPro gives larger nocturnal spectral correction factors respect to EddyUH (see section 4.1 and Fig 4).

3.4 Differences between cumulative fluxes

Mostly the cumulative sums of not gap filled flux time series are within ±2 %, which suggests that there is no significant systematic bias between the two software packages (Table 3). Biggest relative differences were in LI-7700 F_{CH4} and LI-7500 H_2O flux cumulative sums, -6.7 % and -5.3 %, respectively, meaning that the cumulative values estimated with EddyPro were somewhat larger than with EddyUH. For LI-7700 F_{CH4} if the sensor separation correction was omitted the relative difference was 1.0 % (EddyUH fluxes larger). The smallest relative difference was obtained for G1301-f cumulative F_{CH4}, 0.03 %.

The absolute differences between the cumulative CH_4 fluxes at Siikaneva fen during period May-June 2010 were -0.02 g(CH_4) m^{-2} (LI-7700, EddyPro larger) and less than 0.01 g(CH_4) m^{-2} (G1301-f) (Table 3). The difference between cumulative CO_2 fluxes was -4 g(CO_2) m^{-2}, EddyUH was showing slightly higher CO_2 uptake. This originated from the fact that EddyPro estimated approximately 1-3 % higher respiration at night and EddyUH calculated <1 % higher uptake during daytime (cf. Fig. 4e). These differences were caused by the spectral corrections and they inflicted the observed deviation between the cumulative LI-7000 CO_2 fluxes. At the Erottaja urban site during July-September 2010 EddyUH showed slightly lower cumulative CO_2 emission (-2 g(CO_2) m^{-2}) for LI-7200, whereas for LI-7500 the difference was clearer (-27 g(CO_2) m^{-2}). Similarly as in the case of LI-7000 CO_2 fluxes, also here the difference observed between LI-7500 cumulative F_{CO2} was likely caused by the spectral corrections (cf. Fig. 4i). The cumulative H_2O fluxes were within 2 mm. However, the data coverage should be considered when evaluating the significance of these absolute differences. The data coverage of the Siikaneva measurements was between 73 % (CH_4, G1301-f) and 21 % (CH_4, LI-7700). At the Erottaja site lower data coverage was obtained (between 37 % (CO_2, LI-7500) and 29 % (H_2O, LI-7500 and LI-7200)).

4. Discussion

We have performed an inter-comparison between EddyUH and EddyPro, two public software packages for EC flux calculation. Both software's feature up to date methods for EC rawdata processing steps and corrections. Flux data as estimated by the reference combinations (Table 2) were in good agreement. In general, there were not significant systematic differences in the un-corrected fluxes calculated by EddyUH and EddyPro (Fig. 4). This suggests that an optimal choice for the raw data preparation and processing schemes leads to avoid systematic biases in the fluxes between the two software packages. The most significant differences between the softwares were after the flux corrections, as discussed next for closed and open path systems.

4.1 Critical steps and recommendations for closed-path systems

EC measurements from three closed-path systems (LI-7000, LI-7200 and G1301-f) were processed and the impact of different processing step combinations was analysed using runs performed with EddyUH and EddyPro. Among the different calculation procedures analysed, the spectral correction was the most relevant for the closed-path LE measurements at the two sites, the median values being between 6% and 16%. On average, the use of theoretical spectral correction gave up to 6% lower LE in Erottaja, while in Siikaneva the deviation respect to the reference run was generally below 3%. We determined a stronger RH dependence of low pass filter time constant in Erottaja than in Siikaneva (Fig. 8) caused by the non-heated sampling line there (Nordbo et al., 2013). Moreover, the low pass filter time constants estimated by EddyPro in Erottaja were larger than those estimated by EddyUH for RH values lower than 80% (Fig.8c). This may explain the 2% difference between LI-7200 LE as estimated by EddyPro and EddyUH (Fig. 3g). Although these values are not directly comparable with other studies, they are in the same range previously reported (Fig. 2). Surprisingly, at Siikaneva the theoretical spectral correction gave on average 7% higher F_{CO2} and F_{CH4} than the experimental spectral correction, and the result was consistent between the software packages. A possible explanation could be that in the site-specific co-spectral model used in the reference run, the cospectral peak frequency n_m = 0.056 estimated in unstable conditions is shifted to lower frequencies respect to the Kaimal et al. (1972) based atmospheric surface layer (ASL) cospectral model used in the theoretical spectral correction (Moncrieff et al., 1997). In addition in stable conditions the stability dependence of the estimated n_m is less pronounced, and it does not follow strictly the ASL parameterization (data

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
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not shown). This would result in smaller spectral corrections when using the site-specific cospectral model in Eq. (B2). In addition, we found that in Siikaneva the LI-7000 F_{CO2} was greatly affected by the dilution effect due to the wet surface conditions and the presence of vegetation at the site producing large H_2O fluxes (average daytime value of LE equals 170 W m^{-2}). The same correction affected less F_{CH4} measured by G1301-f, because the flux to concentration ratio for CH_4 was larger than the one for CO_2. In Erottaja the same effect on F_{CO2} measured by LI-7200 was much lower (on average 2%), because of the three times smaller daytime values of LE at this urban site. Besides this, the sampling line was not heated in Erottaja, and different magnitude of the dilution correction between the two sites was expected. In fact, although the heating (and insulation) of the sampling line decreased the H_2O low pass filter effect (especially at increasing values of RH), at the same time it increased the H_2O fluctuations in the sampled air, leading to larger dilution correction. It is common to think that the density and spectroscopic corrections have small importance for closed-path analysers, since the temperature fluctuations are dampened in the sampling tube (Leuning and Judd, 1996; Rannik et al., 1997). However, as we have demonstrated here, this depends on the ecosystem type and system setup. Fortunately, current closed-path gas analysers report also H_2O turbulent signals, and the measured gas mole fractions can be readily converted into dry mole fractions either in the analyser internal software or in the post-field rawdata processing.

Finally for our sites and datasets the use of nominal constant time lag was an issue only for nocturnal LE, when the absorption effect on H_2O in the sampling line became more relevant, determining an increase of H_2O time lag, and a 3% and 2% flux underestimations in Erottaja and Siikaneva respectively (see Figs. 6d and 7b). Daytime deviations were very small because of the strategy adopted for searching the H_2O time lag (see Appendix A).

4.2 Critical steps and recommendations for open-path systems

Open-path analysers measure the gas molar densities in open measurement cell and thus, if not properly corrected, the temperature and humidity fluctuations in the open cell may cause apparent surface fluxes to be measured. For open-path analysers the WPL correction terms can often surpass the magnitude of the flux itself and also change the sign of the measured target gas flux (e.g. Peltola et al., 2013). Since the correction is additive, meaning that its magnitude does not depend on the flux itself, its relative importance increases significantly when small fluxes are measured. Thus it is critical to perform this correction accurately, especially when small fluxes co-occur with large H and LE fluxes. The correction should be done using H and LE actual values, meaning fully corrected fluxes, and in this case the iteration loop includes more steps respect to closed-path systems (Fig. 2). Any bias in the correction routines to H or LE will propagate through the WPL correction to bias the flux estimate. Lee and Massman (2011) showed that in an ordinary situation 2 % error in H spectral corrections will result in 40 g(CO_2) m^{-2} bias annually. However, the WPL correction is based on unambiguous physical laws and if correctly implemented it does not bias the resulting fluxes.

If the response time which characterises the measurement system ability to measure flux contribution of small eddies, i.e. high frequencies, is determined using power spectra, then the high frequency dampening caused by spatial sensor separation needs to be estimated separately. In EddyPro it was done using the method proposed by Horst and Lenschow (2009), while EddyUH uses cospectra to estimate the measurement system's high frequency response and thus no additional correction for sensor separation is needed. The Horst and Lenschow (2009) method is based on cospectral peak frequency (n_m) parameterisations against the stability parameter ζ, in addition to ASL cospectral model (as presented in Horst (1997)). Using these assumptions, they derived a dependence between the signal dampening due to sensor separation and the cospectral peak wavenumber and sensor separation in crosswind, along-wind and vertical directions.

For LI-7700 at Siikaneva site, it was shown that this correction resulted in systematic differences between the softwares (Sect. 3.4) and between the two co-located CH_4 instruments (Sect. 3.2). The correction method seemed to overcorrect LI-7700 CH_4 fluxes, which resulted in too high CH_4 fluxes. As mentioned above the correction method relies on n_m vs ζ parametrisations and Horst (1997) cospectral model and if these do not comply with the spectral characteristics of turbulence observed at the site, then the correction will be biased. Furthermore, LI-7700 was situated significantly below the sonic anemometer (0.45 m) when compared with the sonic measurement height (2.75 m) and possibly, in such case, the correction method does not perform well. Nevertheless, the difference observed in this study emphasises the need for accurate spectral corrections and the importance of minimising the sensor separation when constructing an EC measurement setup. The sensor separation corrections are especially important for open-path analysers, since they cannot be mounted very close to the sonic anemometer due to their size and the flow distortion they may create.

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

5. Conclusions

We have estimated and analysed the flux uncertainty due to the use of two software packages, using two and three months long datasets including CO_2, CH_4 and LE fluxes measured over a wetland and an urban site in Finland, respectively. Outputs from EddyUH and EddyPro, two popular software packages for post-field processing of eddy covariance data, were compared. We evaluated the most critical processing steps, determining the largest deviations in the calculated fluxes. We found that the raw data preparation and processing steps were consistent between the software packages, and most of the deviations in the estimated fluxes were due to the flux corrections. Among the different calculation procedures analysed, the spectral correction was the most relevant for closed-path LE fluxes, reaching a night-time median value of 15% at the wetland site. We found up to 43% deviation (with respect the reference run) if closed path CO_2 flux is calculated without the dilution correction, while the CH_4 fluxes were up to 10% lower without dilution and spectroscopic corrections. The density (and spectroscopic) correction was the most critical step for open-path systems. However, we found also large spectral correction factors for the open-path CH_4 fluxes, due to the sensor separation effect. Turbulent fluxes calculated with a reference combination of processing steps were in good agreement, being the systematic difference between the two software packages up to 2% and 6.7% for half-hour and two months cumulative sum values, respectively. This result is an improvement with respect to earlier software inter-comparison studies (e.g. Mauder et al., 2008), and it suggests that a consistent choice of implemented methods for the post-field processing steps can minimize the systematic flux uncertainty due to the usage of different software packages. Finally, it is recommended in the future to work towards more software inter-comparison studies, where new methods and corrections are validated across different type of ecosystems, including those where the flux signal to noise ratio is rather small.

Appendix A: Raw data preparation and processing in EddyUH

In the first level of data processing several operations are done to the raw dataset in order to calculate un-corrected covariances of interest. Several methods related to these processing steps are available (see Table 1), and they are shortly presented below.

Quality control and despiking. The raw data are quality flagged according to physical plausible ranges of high frequency values of each variable, diagnostic parameters (if available), and several tests as described in Vickers and Mahrt (1997). Further spikes are then detected and commonly this is done applying the Vickers and Mahrt (1997) method. However also other methods exist in EddyUH, e.g. the difference limits method, which compare the difference between consecutive data points to given threshold for each raw data time series (see Rebmann et al., 2012 for more details). If the time series contains too many spikes, the data might be useless and a flux should not be calculated for the averaging period of interest (commonly 30 min). Foken (2008) suggests excluding time series with more than 1 % spikes from further analysis.

Dilution and spectroscopic corrections. Current closed-path gas analysers measure H_2O inside the sampling cell making the conversion of gas mole fraction relative to dry air possible through a point-by-point dilution correction. In addition, H_2O affects the shape and width of an absorption line used to estimate gas concentration via pressure broadening. This cross-interference can be corrected with the so-called spectroscopic correction (e.g. Peltola et al., 2014). Many of the new laser based gas analysers output dry mole fraction (mol $mol_{dry\ air}^{-1}$) and thus no dilution or spectroscopic corrections are needed during data post-processing. However, for older gas analysers these corrections are needed.

Coordinate rotation. A coordinate rotation is applied to the wind velocity components, in order to align the x-axis parallel to the mean wind direction and to set the mean vertical velocity equal to zero. This is done according to common practice with two alternative approaches, the so-called 2D rotation (Rebmann et al., 2012) or the sector-wise planar-fit (PF) method (Wilczak et al., 2001).

Calculation of turbulent fluctuations. In order to extract the turbulent fluctuation from the measured time series, the time series need to be detrended by subtracting the mean part. There are three methods available in EddyUH, i.e. block averaging, linear detrending and autoregressive filtering (Rebmann et al., 2012). Of these three detrending methods only block-averaging fulfils the Reynolds averaging rules. All the detrending methods attenuate the low-frequency part of the cospectra. Block-averaging has the smallest effect on the cospectra, whereas autoregressive filtering attenuates the cospectra the most (Rannik and Vesala, 1999). Autoregressive filtering may be a good detrending method if the instrument used creates unwanted variation in the signal, as in Mammarella et al. (2010). However, often block-averaging is recommended.

Crosswind correction of sonic temperature. Sonic anemometers calculate sonic temperature T_s based on three paths and thus crosswind should be taken into account. The correction can be applied point by point to the temperature fluctuations (Liu et al., 2001 eq. 10) or to the

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

Atmospheric Measurement Techniques Discussions

temperature covariance (Liu et al., 2001 eq. 12). Note that some sonic anemometers might include this correction in their internal firmware.

Time lag determination and adjustment. The gas signal measured by closed-path analysers usually lags the wind speed measurement made with sonic anemometer. The time lag can be estimated theoretically if sampling tube length and diameter are known, in addition to flow rate in the tube. However for H_2O the time lag depends on relative humidity due to adsorption and desorption of water on the tube walls (Ibrom et al., 2007a; Mammarella et al., 2009; Massman and Ibrom, 2008). Lag between open-path gas analyser measurement and sonic anemometer measurement is caused by the sensor separation: the further away the gas analyser is from the anemometer the longer the time lag between the two measurements is. It also depends on wind speed and direction. The time lag (for both open- and closed path systems) is commonly determined by searching the maximum of cross-covariance between the vertical wind and gas signal time series within a certain predefined lag window. With this method effects of slightly varying flow rate and relative humidity on H_2O time lag can be properly taken into account. The used lag window should be as narrow as possible; however it should be wide enough in order to cover the variation in time lag during the processed period. In EddyUH a constant search window is used through the whole measurement period for CO_2 time lag estimation, whereas for H_2O the lag window boundaries vary as a function of relative humidity (Clement, 2004; Nordbo et al., 2012). First, the boundaries for H_2O need to determined by allowing the H_2O signal to have a clearly wider lag window than CO_2. Hence, a variable and narrower search window is determined and the H_2O time lag estimated again (time lag optimization).

Finally, covariances are calculated as a final step of the first processing level, which is performed by the pre-processor in EddyUH. Besides covariances and time lag estimates, the EddyUH pre-processor outputs include wind and gas signals statistics (mean, standard deviation, skewness, kurtosis), power spectra and co-spectra for each averaging time period. In addition, quality statistics parameters are also calculated, e.g. flux steady-state and integral turbulence characteristics (Foken and Wichura, 1996), instrumental noise (Lenschow et al., 2000) and random flux error (Finkelstein and Sims, 2001). All these data are saved in monthly binary files, and then used by other modules (Fig.1).

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

Atmospheric Measurement Techniques Discussions
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Appendix B: Corrections to the covariances in EddyUH

In the second level of processing, several corrections must be applied to the 30 min covariances, and the set of corrections are different for closed and open-path systems (see Fig. 2). At this stage the estimated co-variances are used to calculate the stability parameter defined as

$$\zeta = \frac{z-d}{L} = (z-d)\left(-\frac{T_p u_*^3}{g\kappa \overline{w'T_s'}}\right)^{-1}, \tag{B1}$$

where z is the measurement height (m), d the displacement height, (m), L the Obukhov length (m), T_p the potential temperature (K), $u_* = \sqrt[4]{\overline{u'w'}^2 + \overline{v'w'}^2}$ the friction velocity (m s^{-1}), g the acceleration due to the gravity (m s^{-2}) and κ the von Karman constant.

Spectral correction. Flux loss at high frequency is due to the incapability of the measurement system to detect small scale variation. The inadequate frequency response, sensor separation, line averaging and, in closed-path system, the air sampling trough tubes and filters are the main reasons causing co-spectral attenuation. On the other hand, flux loss at low frequency is due to limited averaging period (30 min) and trend removal. The frequency response correction is usually performed based on a priori knowledge of the system transfer function and the un-attenuated cospectrum, e.g.

$$F_c = \frac{\int_0^\infty C_{ws}(f)df}{\int_0^\infty TF(f)C_{ws}(f)df} \quad . \tag{B2}$$

Here F_c is the estimated spectral correction factor, C_{ws} the normalized un-attenuated cospectrum, f the frequency and $TF=TF_H{\cdot}TF_L$ the total transfer function. The correction always increases the flux. The low frequency correction depends on the used detrending method (see Appendix A), and is performed using theoretical derived formulations for TF_L (Rannik and Vesala, 1999).
The high frequency transfer function TF_H can be derived either theoretically or experimentally (Foken et al., 2012). The correction is different for momentum flux, sensible and latent heat fluxes, other gas fluxes and it differs between open- and closed-path EC systems. In the theoretical approach, the ASL co-spectral models (Moncrieff et al., 1997) are used and TF_H is

calculated as superposition of specific transfer functions representing different causes of flux loss, whose formulas can be found in (Leuning and Judd, 1996; Moncrieff et al., 1997; Moore, 1986). This approach works fine for correcting the momentum and sensible heat flux, as well as for gas fluxes measured by open-path systems. Alternatively the experimental approach can be used, where the model co-spectra and TF_H are estimated using in situ measurements. Different methods have been proposed for retrieving the TF_H from the measured power spectra or cospectra of T_s and the target gas dry mole fraction (Fratini et al., 2012; Ibrom et al., 2007a; Mammarella et al., 2009; Nordbo et al., 2014). In EddyUH the method by Mammarella et al. (2009) is included. Many studies have used the theoretical approach because it is simpler to apply, while the experimental approach requires site and sensor-specific investigations.

Density correction. For measurements done with an open-path gas analyser, fluctuations in air density cause apparent variations in measured scalar concentration and this needs to be corrected (WPL correction) according to Webb et al. (1980). The correction is performed to 30 min fluxes of the target gas, and the humidity and temperature covariances used in the correction should correspond to situations in ambient air, e.g. fully corrected. For closed-path gas analyser the correction can be done to the covariances as well as an alternative of dilution correction applied to the raw data. The correction is more simple than for open-path gas analyser due to the fact that the temperature fluctuations are usually dampened in the sampling line (Rannik et al., 1997). Then only H_2O fluctuations are relevant and it is preferable that H_2O is measured in the same cell as the gas whose flux is corrected, similarly as in dilution correction. If this is not the case then external H_2O measurements can be used, and the H_2O covariance, should be modified to correspond to circumstances in the measurement cell (Ibrom et al., 2007b; Peltola et al., 2014).

Spectroscopic correction. Gas density measurements carried out with instruments whose measurements are based on laser spectroscopy (like LI-7700 and G1301-f analysers), require also corrections for spectroscopic effects that affect measured values, in addition to the above mentioned density corrections. As these spectroscopic effects are related to the changes in shape of the absorption line due to the changes in gas temperature, H_2O and pressure, one can incorporate the spectroscopic effects into WPL terms (modified equation) (McDermitt et al., 2011).

When estimating the CH_4 fluxes using the LI-7700 one should always use the temperature coming from the sonic anemometer and not those recorded by the in-path thermocouple of the LI-7700 instrument. Furthermore, one should always use the uncorrected CH_4 molar density (mmol

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

Atmospheric Measurement Techniques Discussions

m^{-3}) for flux measurements, while H_2O fluxes necessary to compute CH_4 fluxes should be acquired with an H_2O analyser (in our study LI-7000).

For closed-path systems measuring H_2O in the same sampling cell, it is simple to do the correction to the raw data point-by-point (see above). In case H_2O is not measured internally, it is preferably to dry the air samples or to have external H_2O measurements. In the latter case the correction can be applied to the half-hourly averaged fluxes according to the method proposed by Peltola et al. (2014).

Humidity Correction of Sonic Temperature. The correction is based on the transformation of sonic temperature (T_s) to actual air temperature (T). In EddyUH, the updated version (van Dijk et al., 2004) of the original Schotanus et al. (1983) correction is implemented. Following the derivation in van Dijk et al. (2004) the temperature covariance is calculated as

$$\overline{w'T'} = \left(1 - 0.51\bar{q}\right)\overline{w'T_s'} - 0.51\bar{T}\,\overline{w'q'}, \qquad \text{(B3)}$$

where $\overline{w'T_s'}$ and $\overline{w'q'}$ are the final sonic temperature and H_2O covariances (e.g. after spectral correction) and q is specific humidity (kg(H_2O) kg(moist air)$^{-1}$). The covariance $\overline{w'T'}$ is then used in Eq. 3 to calculate H, while the covariance $\overline{w'T_s'}$ is used to recalculate the stability parameter in Eq. B1.

Corrections to the covariances are repeated in an iteration loop until the flux change is smaller than 0.01% (see Fig. 2). In EddyUH these steps are performed in the "Flux calculation" module, including the estimates of flux density according to the Eqs. [1-4].

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Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
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Table 1. List of implemented methods for data processing in EddyUH.

Raw data preparation and processing	**Implemented methods**
Quality control and spike detection	Raw data quality tests (Vickers and Mahrt, 1997), diagnostic flags. Several despiking methods (Rebmann et al., 2012)
Conversion to dry mole fraction	Dilution and spectroscopic correction point by point.
Calculation of turbulent fluctuations	Block averaging, linear detrending and autoregressive running mean filter (Rebmann et al., 2012)
Coordinate rotation	Sector-wise planar fit (Wilczak et al., 2001), 2D rotation (Rebmann et al., 2012)
Crosswind correction of sonic temperature	Liu et al.(2001)
Time lag determination	Constant time lag, Cross-covariance maximization, Time lag optimization
Quality statistics	Flux steady-state and integral turbulence characteristics (Foken and Wichura, 1996), instrumental noise (Lenschow et al., 2000) and random flux error (Finkelstein and Sims, 2001).
Corrections to the covariances	**Implemented methods**
Calculation of stability parameter	Eq. (B1)
High frequency loss	Theoretical method (Moncrieff et al., 1997). Experimental method, e.g. empirical estimation of TF_H and co-spectra model (Mammarella et al., 2009)
Low frequency loss	Rannik and Vesala (1999)
Humidity correction of sonic temperature	van Dijk et al. (2004)
WPL correction	Based on Webb et al. (1980) for open-path and Ibrom et al. (2007b) for closed-path gas analysers.
Spectroscopic correction	Based on McDermitt et al. (2011) for open-path and Peltola et al. (2014) for closed-path gas analysers.

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

Table 2. Software setups for the reference combination.

Processing steps\Software	**EddyUH**	**EddyPro**
Despiking	Difference limit (Appendix A)	Vickers and Mahrt (1997)
Conversion to dry mole fraction (for closed-path)	Yes	Yes
Detrending	Block averaging	Block averaging
Coordinate rotation	2D ($\overline{v} = \overline{w} = 0$)	2D ($\overline{v} = \overline{w} = 0$)
Crosswind correction	Yes, according to Liu et al. (2001)	Yes, according to Liu et al. (2001)
Time lag estimation and adjustment	Max cross-covariance with time lag optimization	Max cross-covariance with time lag optimization
Spectral correction	Yes, according to Mammarella et al. (2009)	Yes, according to Fratini et al. (2012)
Density correction to 30 min fluxes (only for open-path)	Yes, according to Webb et al. (1980)	Yes, according to Webb et al. (1980)
Spectroscopic correction	For LI-7700 F_{CH4} according to McDermitt et al. (2011). For G1301-f F_{CH4} according to (Rella, 2010)	For LI-7700 F_{CH4} according to McDermitt et al. (2011) Correction for closed-path is not implemented.

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

Atmospheric Measurement Techniques Discussions

Table 3. Cumulative sums estimated with EddyUH and EddyPro. Relative differences and data coverage are also shown. Data were not gap-filled prior to calculation of the cumulative sums.

	Siikaneva fen (May-June 2010)						Erottaja urban site (July-September 2010)			
	F_{CH4} (g m-2)			F_{CO2} (g m-2)	ET (mm)		F_{CO2} (g m-2)		ET (mm)	
	G1301-f	LI-7700	LI-7700[1]	LI-7000	G1301-f	LI-7000	LI-7200	LI-7500	LI-7200	LI-7500
EddyUH	2.25	0.26	0.26	-126	137	127	1060	1039	30	30
EddyPro	2.25	0.27	0.25	-122	135	127	1062	1066	30	31
(EddyUH-EddyPro)/EddyPro	0.03 %	-6.7%	1.0 %	3.3 %	1.5 %	1.3 %	-0.2 %	-2.5%	0.7 %	-5.3%
Data coverage	73%	21%	21%	61%	71 %	69 %	37%	37%	29 %	30 %

[1] No sensor separation correction in EddyPro.

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

Atmospheric Measurement Techniques
Discussions

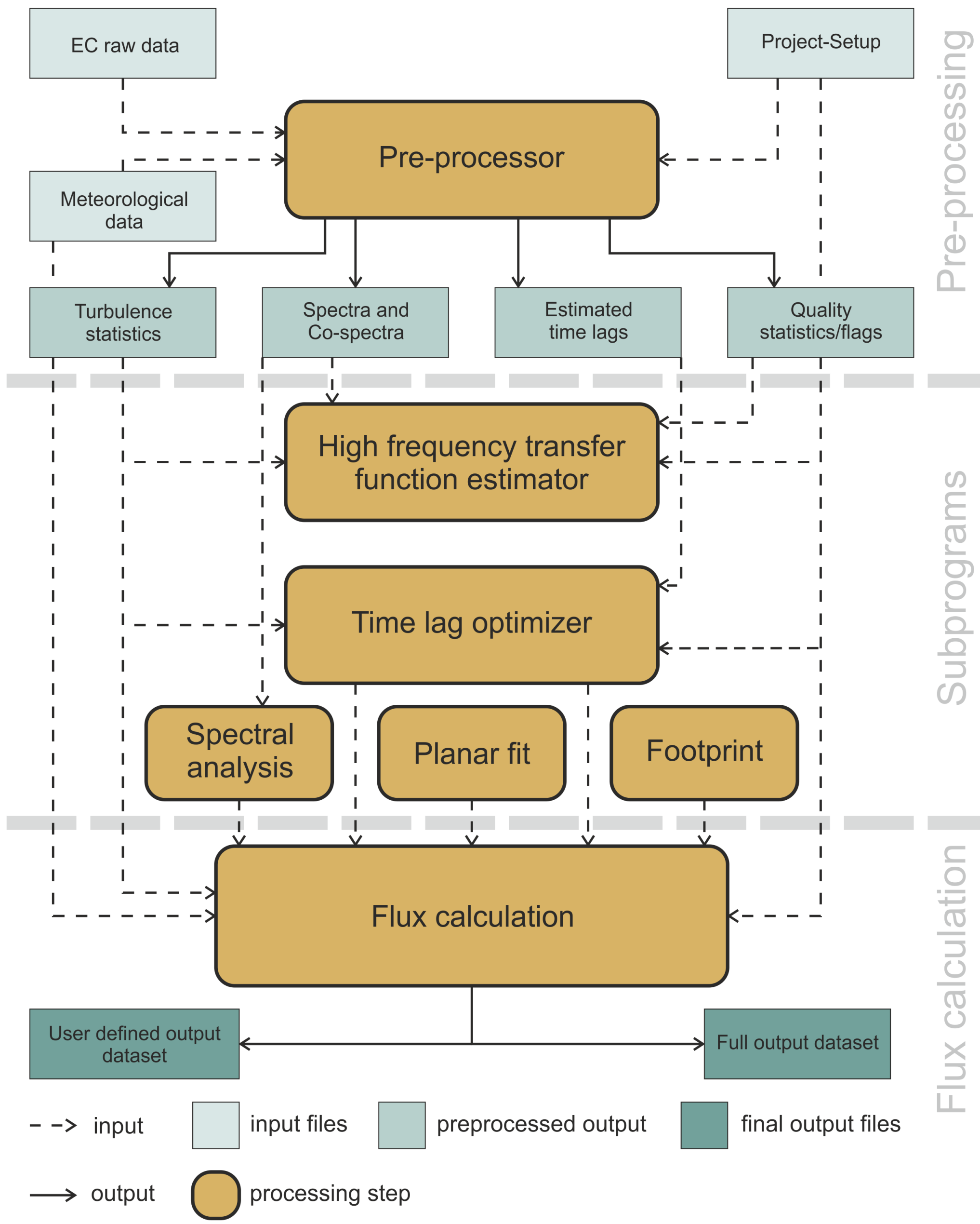

Figure 1 Flow chart of EddyUH.

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

Atmospheric Measurement Techniques
Discussions
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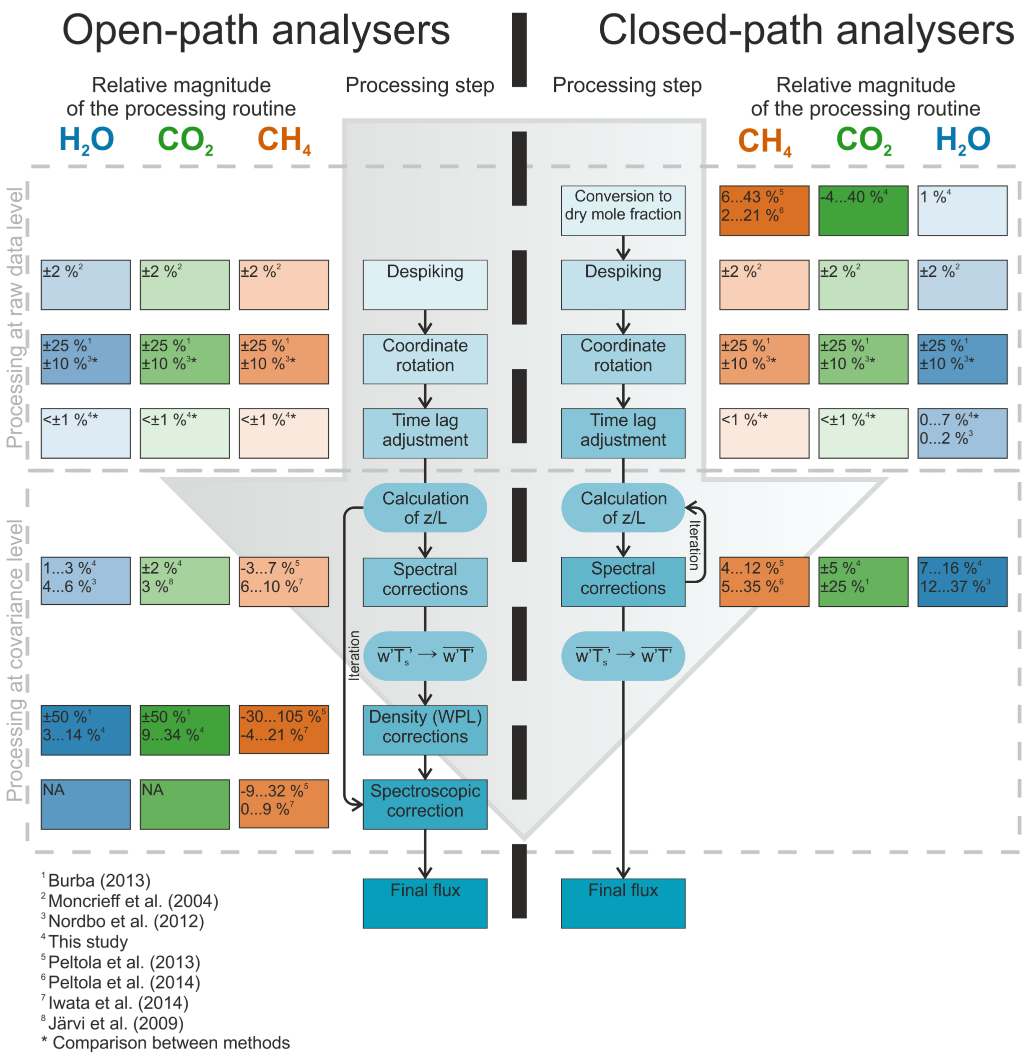

Figure 2. EC data processing scheme for open- and closed-path gas analyser data. Relative magnitude of each processing step is also reported, according to this and other studies. Negative values mean that the correction increases downward fluxes, and positive values correspond to correction increasing upward fluxes.

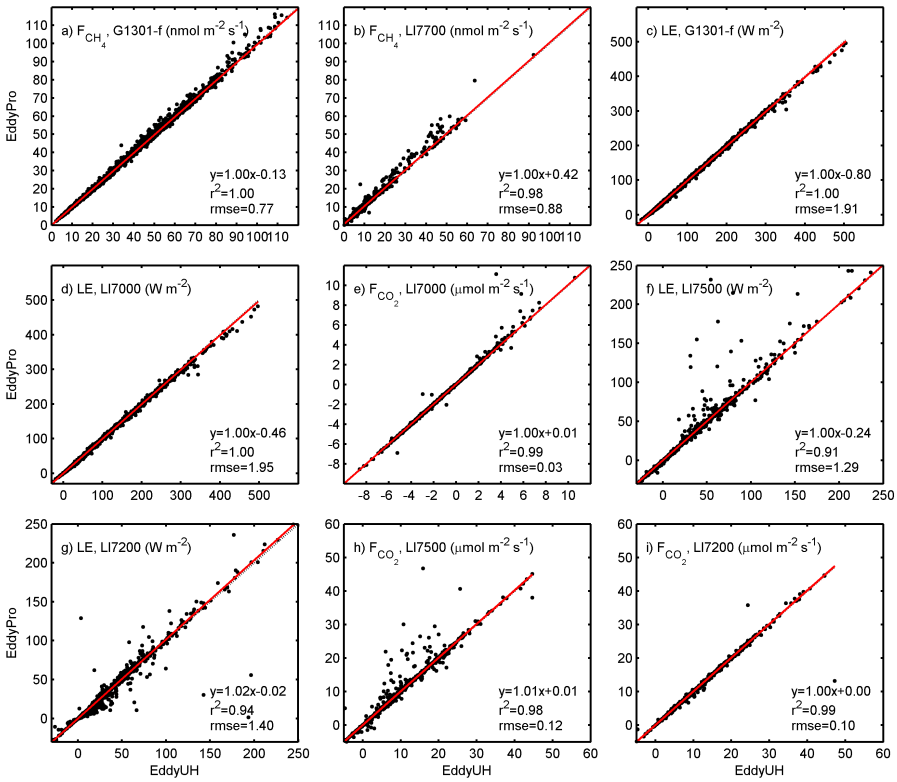

Figure 3. Comparison of the reference run fluxes estimated by EddyUH and EddyPro. CH_4 flux measured by G1301-f (a) and LI-7700 (b), LE measured by G1301-f (c) and LI-7000 (d), CO_2 flux measured by LI-7000 (e), LI-7500 (h) and LI-7200 (i), and LE measured by LI-7500 (f) and LI-7200 (g). Each dot represent a 30 min data value. Dashed lines indicated the 1:1 line and red solid lines the linear regression to the data.

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

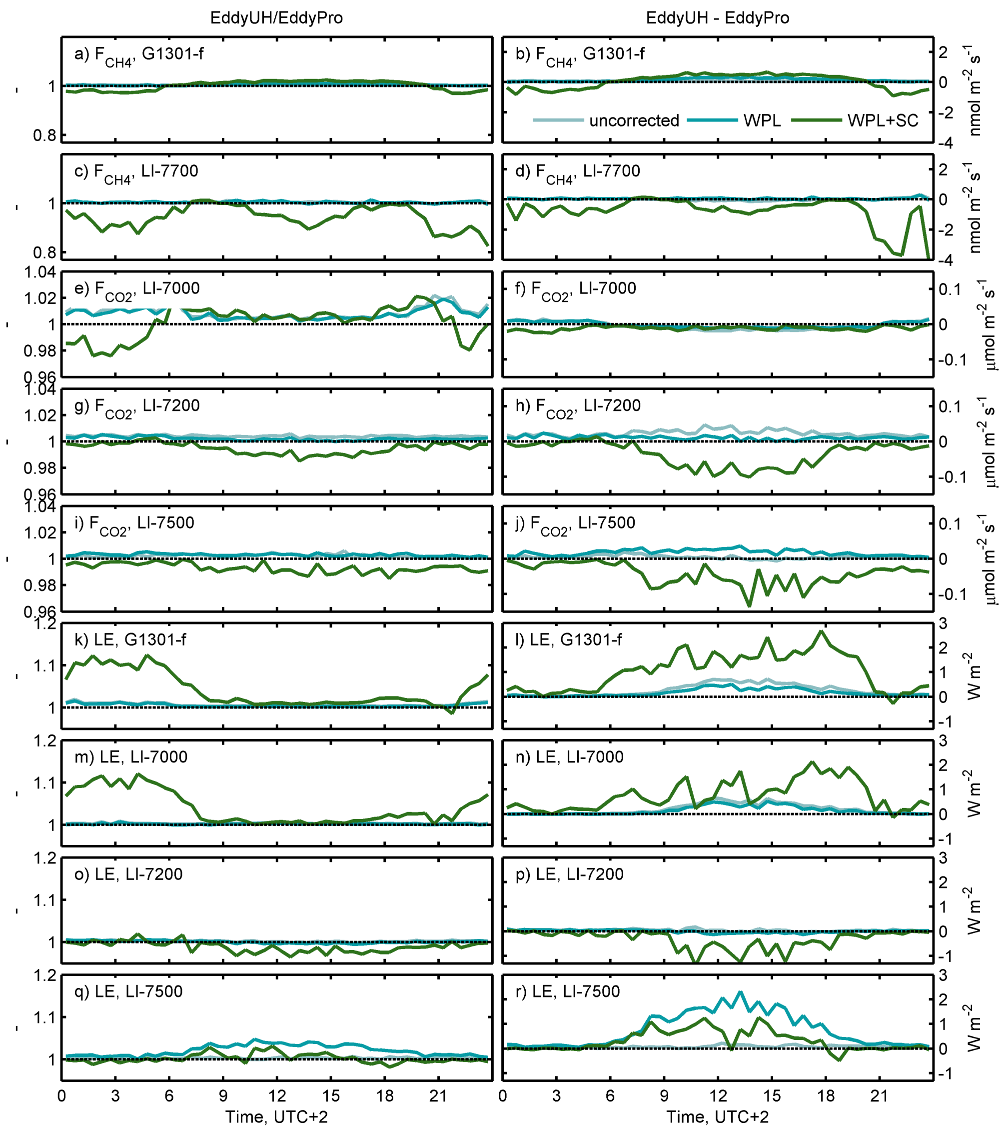

Figure 4. Median diurnal variation of flux ratio (left side) and bias (right side) for the studied instruments and variables between the two software. Light blue shows the uncorrected fluxes after despiking, coordinate rotation, detrending and time lag compensation; blue the WPL corrected fluxes (for G1301-f and LI-7700 F_{CH4} this includes also spectroscopic correction); and green line the WPL plus spectral corrections (WPL+SC) The WPL+SC curves represent data from the reference run, i.e. fully corrected.

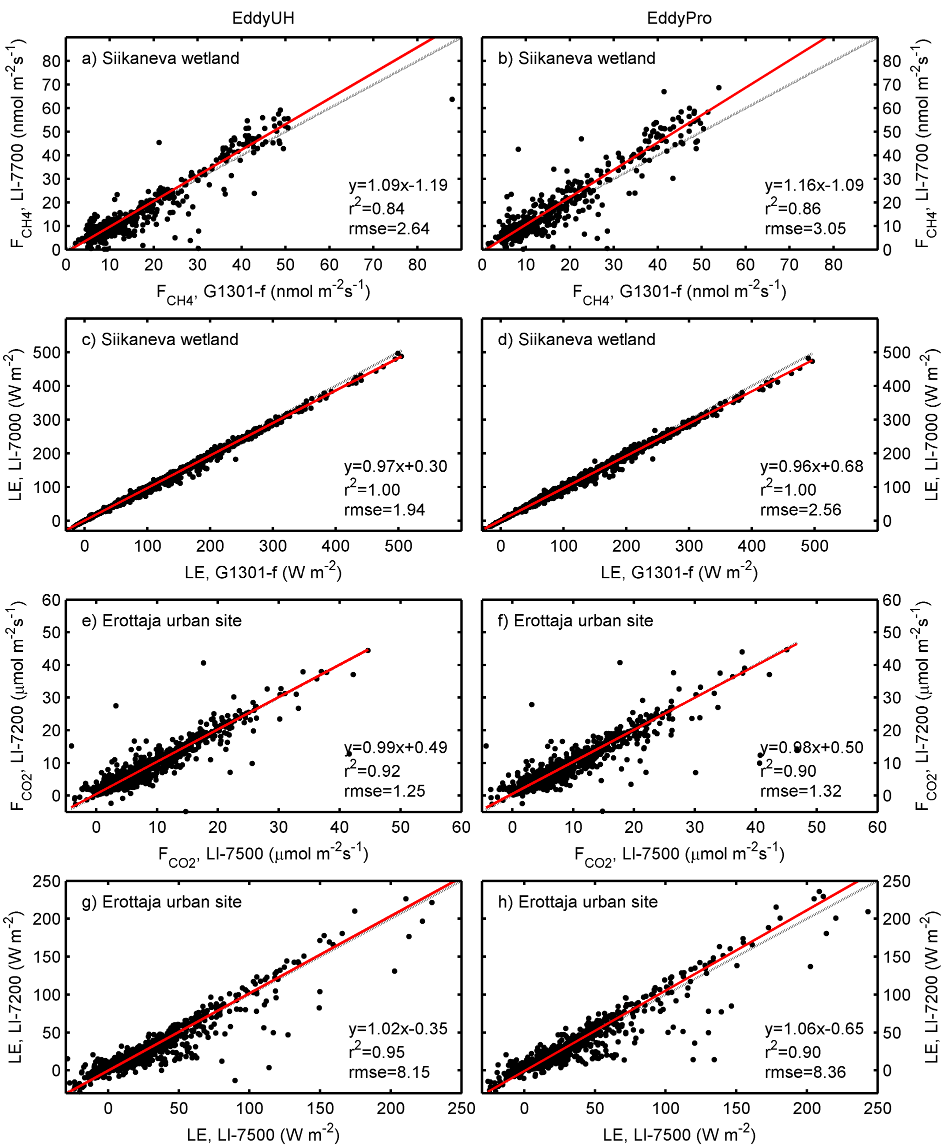

Figure 5. Scatter plots of F_{CH4} measured by G1301-f and LI-7700 (a, b), LE measured by G1301-f and LI-7000 (c, d), F_{CO2} measured by LI-7500 and LI-7200 (e, f), and LE measured by LI-7500 and LI-7200 (g, h). Subplots in the left column show fluxes calculated with EddyUH, and those in the right column fluxes calculated with EddyPro. Each dot represent a 30 min data value. Dashed lines indicated the 1:1 line and red solid lines the linear regression to the data.

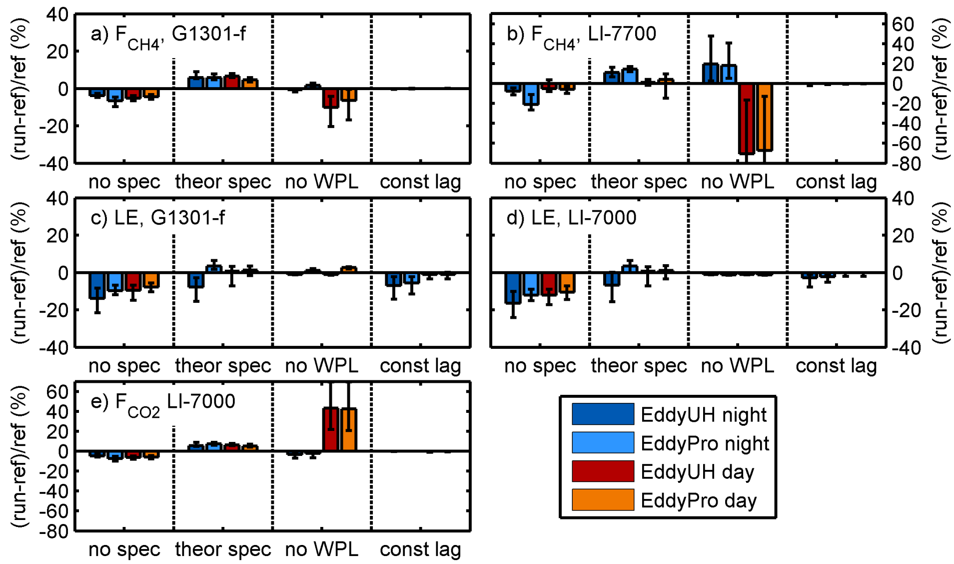

Figure 6. Effect of different calculation procedure of the estimated flux at Siikaneva site, presented as deviation (in %) from the reference run (ref). Deviation is defined as (run-ref)/ref where run refers to the run performed with no spectral correction (no spec), theoretical spectral correction (theor spec), no density and spectroscopic correction (no WPL), and using a constant time lag (const lag). Bars indicate the median values and error bars denote 25th and 75th percentiles. Note the different scale on y-axis in the subplots (b, e) compared to (a, c, d).

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

Atmospheric Measurement Techniques Discussions

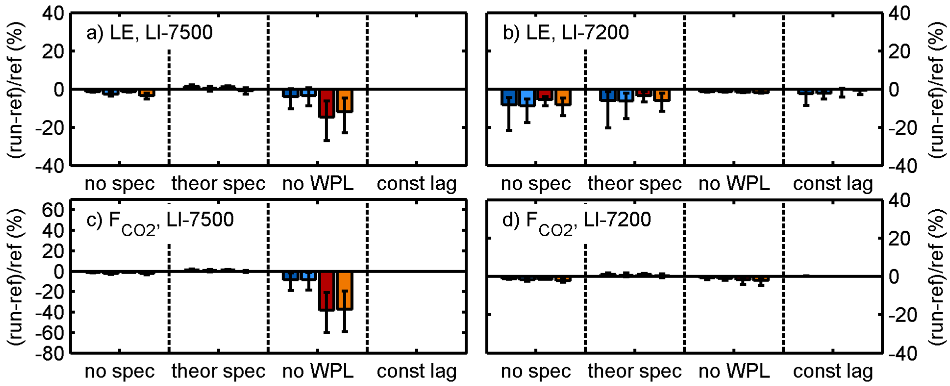

Figure 7. As in Figure 6, but for Erottaja. Note the different scale on y-axis in the subplots (c) compared to (a, b, d).

Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2015-323, 2016
Manuscript under review for journal Atmos. Meas. Tech.
Published: 18 January 2016

Atmospheric Measurement Techniques
Discussions

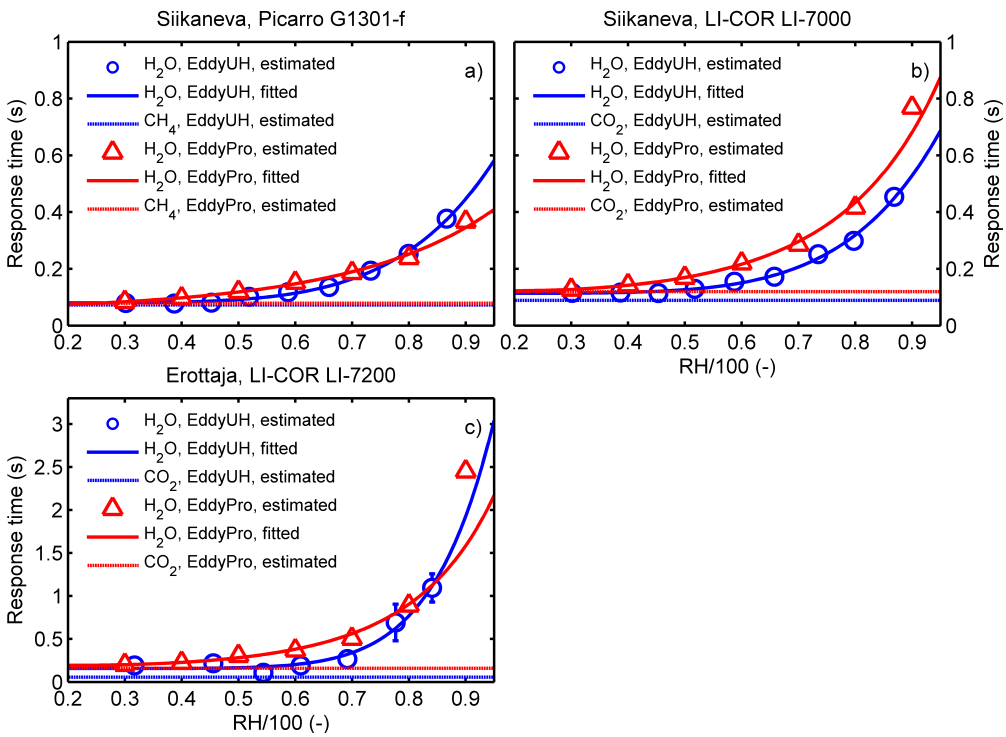

Figure 8. Relative humidity (RH) dependence of low pass filter time constant as estimated with the two software packages. Note the different scale on y-axis in the subplot (c).