



Towards a consistent eddy-covariance processing

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This discussion paper is/has been under review for the journal Atmospheric Measurement Techniques (AMT). Please refer to the corresponding final paper in AMT if available.

Towards a consistent eddy-covariance processing: an intercomparison of EddyPro and TK3

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Received: 17 December 2013 – Accepted: 12 February 2014 – Published: 4 March 2014

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Published by Copernicus Publications on behalf of the European Geosciences Union.

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A comparison of two popular eddy-covariance (EC) software packages is presented, namely EddyPro and TK3. Two about one-month long test datasets were processed, representing typical instrumental setups, i.e. CSAT3/LI-7500 above grassland and Solent R3/LI-6262 above a forest. The resulting fluxes and quality flags were compared. Achieving a satisfying agreement and understanding residual discrepancies required several iterations and interventions of different nature, spanning from simple software reconfiguration to actual code manipulations. In this paper, we document our comparison exercise and show that the two software packages can provide utterly satisfying agreement when properly configured. Our main aim, however, is to stress the complexity of performing a rigorous comparison of EC software. We show that discriminating actual discrepancies in the results from inconsistencies in the software configuration requires deep knowledge of both software packages and of the eddy-covariance method itself. In some instances, it may be even beyond the possibility of the investigator who does not control the source code. Being the developers of EddyPro and TK3, we could discuss the comparison at all levels of details and this proved necessary to achieve a full understanding. As a further consequence, we also suggest that, to the aim of assuring consistency and comparability of centralized flux databases, and for a confident use of eddy fluxes in synthesis studies on the regional, continental and global scale, researchers rely on established software, notably those that have been extensively validated in documented intercomparisons.

1 Introduction

The eddy-covariance (EC) processing sequence to calculate turbulent fluxes from raw, high-frequency data is complex, depending on the chosen instruments, their deployment, the site characteristics, and the atmospheric turbulence peculiarities. The software realizing this processing is analogously complex to develop, maintain and

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7, 2107–2126, 2014

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support. An overview of nine popular software packages including a detailed list of their features is available in Foken et al. (2012). Such official EC software packages are often and repeatedly tested and inter-compared, improved on the basis of users' feedbacks and updated to catch up with new findings and refinements to the EC processing methods. The resulting robustness, quality and reliability are difficult to achieve otherwise.

For our purposes, it is convenient to introduce a nomenclature for the operations performed in EC software. In this paper, a *processing scheme* is the ensemble of all operations performed by the software, from the ingestion of raw data to the calculation of corrected fluxes. A *processing step* is any major operation in the processing scheme, for example the tilt correction or the elimination of spikes. For a given processing step, several *methods* can be available in the literature, and different packages can thus implement a processing step with different methods. Often, a given software supports multiple methods for some of the processing steps, freely selectable by users. It is also to be noted that the same processing scheme can be implemented differently in different packages, because in some cases also the order in which the steps are performed matters. In addition, some software performs iterations of (some) processing steps.

The impact of the entire post-processing typically amounts to 5–20% for energy fluxes and more than 50% for CO₂ fluxes if open-path analyzers are used (Mauder and Foken, 2006). It is therefore not surprising that fluxes obtained from the same raw data processed with different software packages usually do not agree completely. For energy fluxes, Mauder et al. (2007) found an agreement within 10–15% in an intercomparison of six different EC packages from renowned international research institutions, while Mauder et al. (2008) found an agreement within 5–10% of the resulting CO₂ fluxes when comparing seven different software packages used in CARBOEUROPE-IP. The larger discrepancies in the first study occurred because participants had applied different processing schemes, reflecting different opinions on the best way to process those particular datasets. In contrast, all developers of the second study had

followed the same prescribed processing scheme, based on the recommendations of Lee et al. (2004).

Differences in post-processing routines present themselves to the researcher who attempts a software intercomparison as either systematic or random differences in resulting fluxes, which are part of the overall measurement uncertainty and therefore need to be characterized. Richardson et al. (2012) distinguish systematic errors associated with different data processing choices into those that arise from detrending or other kinds of high-pass filtering and those due to the choice of the coordinate rotation method. Moreover, inevitable limitations of instrumentation (e.g. finite time response and averaging volume) require corrections during the post-processing, which may cause additional discrepancies. Instrument-related issues may include spikes, power failure, high-frequency losses and effects of air density fluctuations (Richardson et al., 2012).

Causes for discrepancies during intercomparisons can be conveniently grouped into four classes: (C1) inaccuracies in software setup that lead to unintended differences in the processing schemes; (C2) differences in the methods available in each software, for any given processing step; (C3) differences in the actual implementation of a given method or differences in the order in which processing steps are implemented; (C4) implementation errors (bugs). A certain agreement was reached by the eddy-covariance community as to which processing steps are necessary under which conditions, thus any EC software can be expected to allow the appropriate processing schemes. However, as mentioned earlier, large uncertainty remains as to which method shall be adopted for each step, and which is the correct order in the processing sequence. Furthermore, plenty of arbitrariness is left to the developers as to how to implement a given method, because typically published papers do not describe methods in sufficient technical detail. Finally, refinements of existing methods and new findings continuously arise, which impose updates to EC software, as documented for example by the recent works on effects of humidity in closed-path measurements (Ibrom et al., 2007b; Fratini et al., 2012; Nordbo and Katul, 2013), angle-of-attack effects (Nakai and

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Shimoyama, 2012; Kochendorfer et al., 2012; Mauder, 2013) and flux biases due to errors in concentration measurements (Fratini et al., 2013).

Assuming no bugs in the software, in intercomparisons such as the one described in Mauder et al. (2008), and in general when intercomparisons are carried out by experts on the packages under consideration, causes C1 can be minimized or completely avoided. Thus, discrepancies are only due to the causes C2 and C3, which can only be eliminated – if deemed necessary – through a modification of either software being tested. This is however not the general case. Often, for example when evaluating the possibility of switching to a different software, researchers attempt quick, informal intercomparisons to assess the quality of the new one, only to find that results seldom match to a satisfying degree. As witnessed by the authors, the tendency in this case is to interpret discrepancies as an error in the new software, to which the individual is less accustomed. A deeper investigation, not seldom requiring the intervention of the software developers, often reveals that discrepancies beyond the expectations depicted above are due to causes of class C1. That is, the software configuration was not appropriate to perform a meaningful intercomparison.

Triggered by these considerations, in this paper we present an intercomparison of the two EC software packages EddyPro and TK3, with the threefold aim of: (i) showing that they can give utterly satisfying agreement in calculated fluxes; (ii) identifying the sources of residual discrepancies; (iii) stressing the complexity of performing a fair and rigorous software comparison that highlights genuine discrepancies, which shall eventually be regarded as an ineliminable source of uncertainty. To achieve these aims, we will present the evolution of our comparison, identifying and categorizing the reasons for observed differences, showing how the match improves by elimination of such sources, and discussing residual differences. Note that, while we will occasionally make comments on the suitability of certain implementations, an objective evaluation of alternative methods for the processing scheme that we will identify as sources of mismatches is out of the scope of this work.

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EddyPro (www.licor.com/eddypro) and TK3 (Mauder and Foken, 2011) are two of the most popular EC packages that are freely available, with about 3000 downloads in over 150 countries and more than 870 downloads in more than 53 countries, respectively.

Albeit being available only since 2011, the use of EddyPro is rapidly increasing world-wide, because it is comprehensive, open-source (released under the GPL license), free of charge and user-friendly. EddyPro was firstly released by LI-COR Biosciences Inc. in April 2011 as EddyPro Express 2.0. Its code base builds entirely on ECO₂S (the Eddy Covariance Community Software), an open-source software project started in 2007 at the University of Tuscia (Viterbo, Italy) and partially funded by the IMECC (<http://imecc.ipsl.jussieu.fr/>) and ICOS (www.icos-infrastructure.eu) European projects. Before release, ECO₂S was officially tested in a software intercomparison and results are documented in an IMECC project report. At the time of this writing, EddyPro version 5.1.1 includes various options for each processing step required in the eddy-covariance chain.

The history of TK3 can be traced back over more than twenty years. It started with the program “Turbulenzknecht” which was first used to automatically compute turbulent fluxes in 1989. Its major asset were the elaborate quality assessment routines, which were unique at the time (Foken and Wichura, 1996). After more than ten years of successful application in many micrometeorological field campaigns the software was re-developed from scratch in order to utilize the rapid advancements in computer technology and to allow for automatic processing of much longer data sets up to one year. The resulting TK2 software included all state of the art flux corrections (Lee et al., 2004) and was extensively compared with other publically available EC-software (Mauder et al., 2008). Its updated version TK3 is in continuation of this lineage.

2 Comparison strategy

Two test datasets were selected with the intention to be representative of long-term flux observation setups (see Table 1). They both cover a period longer than one month in

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order to represent different weather conditions during the growing season. The closed-path dataset originates from the Hainich EC station above a beech forest, which was part of the CARBOEUROPE-IP network (Knohl et al., 2003). This system consists of a Solent R3 sonic anemometer (Gill Instruments Ltd., UK) and a LI-6262 closed-path gas analyzer (LI-COR Biosciences Inc., NE, USA) at a measurement height of 45 m. The open-path dataset is from an EC system above a grassland located near Graswang, Germany (Mauder et al., 2013), which is part of the Terrestrial Environmental Observatories network TERENO (Zacharias et al., 2011). The measurement height was 3.1 m and the instrumentation consisted of a CSAT3 sonic anemometer (Campbell Scientific Inc., Logan, UT, USA) and a LI-7500 open-path gas analyzer (LI-COR Biosciences Inc.).

In our comparison, we considered results obtained for friction velocity (u_* , ms^{-1}), CO_2 fluxes (F_C , $\mu\text{mol m}^{-2} \text{s}^{-1}$), latent heat fluxes (LE, W m^{-2}) sensible heat fluxes (H , W m^{-2}), and all corresponding quality flags according to the CARBOEUROPE-IP 0/1/2 scheme (Foken et al., 2004). We intentionally started the comparison with a generic definition of the processing scheme, of the kind that an average user would make. We stress again that, having full control of the software code, we could in principle agree on the finest details at the onset, and have the software provide the exact same results at the first trial (provided the codes are free of bugs), but this would be of little help as it would not replicate any realistic situation. Instead, we strived to simulate the typical starting point of an investigator who attempts an inter-comparison.

After a first *round*, we analyzed the results and refined the comparison in two more rounds, by sorting out all potential causes of class C1, i.e. the eliminable differences due to the configuration of the processing scheme, as well as causes C2 and C3, i.e. differences intrinsic to the software. In a couple of cases this exercise led to a revision/extension of either software, while some differences, assessed as being of class C2 (different methods for the same processing step), did remain and fully account for the residual differences.

We decided to apply two different tilt corrections for the two data sets: double rotation for the open-path system and planar-fit for the closed-path system (Wilczak et al., 2001) in order to test the agreement between the two packages with both methods. In accordance with the recommendations of Aubinet et al. (2012) we agreed on the processing schemes described in Table 2.

3 Results and discussion

The quality of the match between the EddyPro and TK3 was quantified by deriving linear regressions (slope, intercept and r^2) of the scatter plots of individual fluxes. Note that the choice of x and y axis for EddyPro and TK3 in the scatter plots was arbitrary and that – because of the independence of the two datasets – we opted for the symmetric RMA (reduced major axis) linear regression model. Furthermore, we considered the percentage of flux results for which the quality flags matched. Rather than presenting only the result of the last round, in the following we shortly describe results obtained during the three rounds, to highlight the reasons for discrepancies and how we could improve the match in subsequent rounds. What we want to stress here is that some improvements were achieved by better tuning the configurations in order to perform the same operations in both EddyPro and TK3, while other improvements could only be achieved by modifying the source code of either software.

3.1 Closed-path dataset

In the first round, results from the closed-path dataset showed a general close agreement, however accompanied by a significant number of scattering fluxes (Fig. 1). In addition, F_c showed a relatively large systematic bias (9%) and the match of calculated quality flags was very poor: for u_* , LE and F_c , only about 60% of the obtained fluxes received the same quality flag from both packages. Only for H , the agreement was almost 90% already.

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Investigation revealed that one major difference of class C2 was hidden in the despiking processing step. In fact, TK3 implements the robust statistical method of Mauder et al. (2013) based on median absolute deviation (MAD), while the Gaussian statistical method of Vickers and Mahrt (1997) was used in EddyPro. This difference explained the observed scatter. Since the comparison showed that for most of the scattering data points, EddyPro results were less realistic than TK3 results, and since the newer despiking method of Mauder et al. (2013) is believed to be more effective, the same algorithm was implemented in EddyPro. Hence, the scatter was largely eliminated in the second round for all observed fluxes. Changes in the source code of EddyPro were required to make this possible, and the new implementation will be available to EddyPro users as an alternative despiking method in a forthcoming release. In the second round, the agreement between quality flags also slightly improved because of the improved comparability of the two packages after this modification. It is to be noted that the despiking method of Vickers and Mahrt (1997) is highly customizable. Therefore, we could have followed a different strategy and try and fine-tune that method in EddyPro until results matched satisfyingly. However, because of the soundness and simplicity of the MAD method, it was deemed appropriate to implement it in EddyPro and propose it as an option to its users.

Hinted by former experience, in the third round we speculated that the systematic bias in F_c could be related to the WPL term and actually, by a mere matter of communication, we found that TK3 and EddyPro were set to treat the gas concentration data differently. Far from being a special occurrence in our comparison, it is often the case that concentration data are available without a clear indication of whether measurements are expressed as mole fractions (moles of gas per mole of air) or as dry mole fractions (also called mixing ratios, moles of gas per mole of *dry* air), as both units are normally reported as $\mu\text{mol mol}^{-1}$ or ppm (for CO_2) and as mmol mol^{-1} for H_2O . The difference between the two is the dilution effect of H_2O on CO_2 measurements (Webb et al., 1980; Ibrom et al., 2007a). Thus, in this case we confronted ourselves with a difference of class C1, a rather trivial but utterly common difference in the settings. Clearly

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agreeing on the nature of the measurements was sufficient to improve the slope of the F_c regression by 6 %, from 0.91 to 0.97. Interestingly, we noted that this adjustment had a negative effect on LE comparison, which exhibited a slope of 0.99 in the second round, and of 0.97 in the last one. Evidently, the seemingly perfect initial match was the result of systematic differences contributing in different directions and largely offsetting each other.

The differences observed in the calculated quality flags required deeper investigation, and highlighted several differences in the implementation: (i) the steady-state test was evaluated at different stages in the processing scheme; (ii) the quantities involved in the flag definition were slightly different; (iii) the definition of the flag for the integral turbulence characteristics (ITC) was following different references: Foken et al. (2004) in TK3 and Göckede et al. (2004) in EddyPro. The agreement of the quality flags was greatly improved by reconsideration of these aspects in EddyPro. The group of TK3 developers has a long tradition in the definition of these quality flags, thus it was deemed appropriate to adapt EddyPro towards TK3, rather than the opposite. Nonetheless, residual discrepancies remained (up to 20 % for the quality flags of F_c) because difference (iii) was not addressed. It is to be noted that, being both based on peer-reviewed published materials, there is no objective way to define a “better” implementation, so this difference (of class C2) shall be regarded as a source of ineliminable uncertainty. Similarly, minor differences in the actual implementation of the quality flag assessment (class C3) contribute to this uncertainty.

The remaining differences in F_c and LE (about 3 %) are entirely explained by different spectral correction methods. TK3 implements the method of Moore (1986), based on analytical transfer functions. Here, tube-dampening effects were taken into account by a first-order filter transfer function with 2 Hz cut-off frequency and the sensor separation in lateral direction was corrected according to Moore’s transfer function while the longitudinal separation had already been eliminated by the time lag compensation. EddyPro supports several spectral correction schemes, including a few accounting for relative humidity (RH) dependent effects on water vapor fluxes (Ibrom et al., 2007b;

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Fratini et al., 2012). For the current comparison, the method described in Horst (1997) was selected because, among the ones not accounting for RH-effects, it is the only one for which a cut-off frequency of 2 Hz could be prescribed a priori. Effects of lateral separation were accounted for following the method of Horst and Lenschow (2009). For closed-path data, the spectral correction is the last step in the chain (possibly before an iteration of the corrections) thus in this case it was easy to verify that the different correction factors provided by different methods fully explained the residual difference in the F_c and LE which, again, shall be regarded as an intrinsic uncertainty.

3.2 Open-path dataset

The comparison with the open-path dataset benefitted from the experience gained during the previous comparison and from modifications in the settings and revised implementations (namely despiking and quality flags, see Sect. 3.1). As a consequence, during the three rounds with this second dataset we did not observe improvements in the match of quality flags.

During the first round we observed a significant dispersion, particularly for F_c , and a systematic underestimation of F_c and LE in TK3 as compared to EddyPro (Fig. 2). Following discussion highlighted that EddyPro was using barometric pressure (as estimated by site altitude) while TK3 was using pressure data available in the raw data files. That is, we incurred in another discrepancy of class C1, and one worth discussing. The pressure data in the raw files was not accompanied by metadata detailing its meaning, units and relevance to the eddy covariance data. In this situation, the natural way of proceeding in EddyPro is to ignore this data and use barometric pressure instead. More in general, it is good practice to ignore data that are not fully documented. As an example, in a closed-path system a pressure data may refer to, at least, the ambient air or the instrument's cell: interpreting this data in the wrong way would lead to significant systematic biases in fluxes. Seen from the opposite perspective, we suggest always combining raw data with the metadata necessary to correctly interpret it and use it during flux computation.

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Once the software were set to use the pressure data from the raw files in the second round, most of the scatter was eliminated and we were left with systematic differences in F_c and LE of about 5 to 7%. The agreement in quality flags is better than that at the first round of the closed-path comparison with almost 70% matching flags for all fluxes and even 92% matching flags for H .

Similar to the closed-path systems comparison, it was easy to guess that the difference was due to different spectral correction procedure. TK3 used again the correction from Moore (1986), while this time the analytic method of Moncrieff et al. (1997) was used in EddyPro. Different from the closed-path case, however, open-path data presents an additional complication when trying to entangle the effects of different spectral corrections from other potential sources of discrepancies. In fact, in this case the WPL terms – which are additive in nature – must be included *after* all fluxes have been corrected for spectral attenuations, and spectral corrections are thus no longer the last step in the processing scheme. To verify whether the difference in the spectral corrections solely accounted for the whole observed difference, in the third round we artificially modified EddyPro to match on average (i.e., across the whole dataset) the spectral correction factors calculated by TK3. After this operation, any residual systematic difference would have to be attached to the treatment of the WPL terms. Obviously, this manipulation is only possible if one has full control of the software code, while it would be relatively difficult (and error-prone) trying to do the same by proceeding backward from final fluxes.

Results show a largely satisfying agreement, with systematic differences virtually eliminated and limited scatter due to residual differences in the spectral corrections. We note again, however, that such agreement cannot be achieved by the normal user of the software who cannot (or is not able to) modify the source code to force – as we did – the spectral correction factors to match, before the WPL terms are calculated. We also note again that the open-path dataset obtained over grassland was processed using double-rotation while the closed-path dataset obtained above a forest was processed using planar-fit tilt correction. While the double-rotation method has a relatively simple

and unambiguous definition, the planar-fit method is significantly more complex and leaves the developer some degree of freedom as to how to implement it. The good matches achieved with both methods across the two datasets after the three rounds show that TK3's and EddyPro's implementations are consistent, providing a sound cross-validation.

4 Conclusions

We have shown that, when properly configured, the two software packages EddyPro and TK3 provide satisfying, yet not perfect, agreement in calculated fluxes and related quality flags. Initial comparisons highlighted discrepancies that could be eliminated by simply improving communication, exchanging more details on data significance and on the processing scheme. This suggests the importance of a very detailed consensus on EC post-processing to achieve the best possible comparability between fluxes processed by different users, even when using the same software. Achieving further improvement required interventions on the source code, in particular with the implementation of the spike detection algorithm of Mauder et al. (2013) in EddyPro, which is soon to become a standard option also in this software. The spectral correction procedures are quite different between EddyPro (Horst, 1997; Moncrieff et al., 1997) and TK3 (Moore, 1986). This is the processing step that caused the largest, and ineliminable, differences in flux results. Residual differences in quality flags are mostly due to different algorithms used for the well-developed turbulence test (Foken et al., 2004).

From our exercise, we conclude that discriminating among actual implementations errors, intentional differences and inaccuracies in the software configuration is only possible for the investigator who has detailed knowledge of the source code and the ability to apply appropriate changes. The presented comparison did not highlight any obvious bug. All differences observed in the third round are explained in terms of different implementations of the same methods, or to the adoption of different methods. We thus conclude that an exhaustive documentation of how fluxes are calculated from raw

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data should, whenever possible, include explicitly the name of software used. We also warn against ad-hoc software intercomparisons as a means to validate EC software and against the use of in-house scripts that did not undergo systematic quality assurance. In order to assure consistency and comparability of centralized flux databases, we rather suggest researchers to rely on established software packages, notably those that have been extensively validated in documented intercomparisons (e.g., Mauder et al., 2008, and this paper).

Acknowledgements. We wish to thank Mathias Herbst for providing the raw dataset from the Hainich station. M. Mauder's contribution was partly funded by the Helmholtz-Association through the President's Initiative and Networking Fund. TERENO is funded by the Helmholtz Association and the German Federal Ministry of Education and Research.

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Table 1. Overview of the two test data sets, measured variables were wind components u , v and w , sonic temperature T_s , CO_2 and H_2O concentration (either number densities or mole fractions) and air pressure p .

Dataset	closed-path	open-path
Duration	49 days	38 days
Variables	$u, v, w, T_s, \text{CO}_2, \text{H}_2\text{O}$	$u, v, w, T_s, \text{CO}_2, \text{H}_2\text{O}, p$
Instruments	Solent R3/LI-6262	CSAT3/LI-7500
Ecosystem	Forest	Grassland
Measurement height	19 m	3.1 m
Tilt correction	Planar-fit	Double-rotation

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Table 2. Processing scheme for the software intercomparison

Raw data preparation	<ul style="list-style-type: none"> – Elimination of spikes – Elimination of outranged values, based on physical thresholds
Raw data processing	<ul style="list-style-type: none"> – 30 min block averaging – Cross-wind correction as applicable – Coordinate transformations – Time lag compensation (covariance maximization in a predefined window)
Flux correction	<ul style="list-style-type: none"> – Correction for density fluctuations as applicable – Correction for high frequency spectral losses – Humidity correction of sensible heat flux from sonic temperature measurements
QA/QC	<ul style="list-style-type: none"> – According to Foken and Wichura (1996) and Foken et al. (2004)

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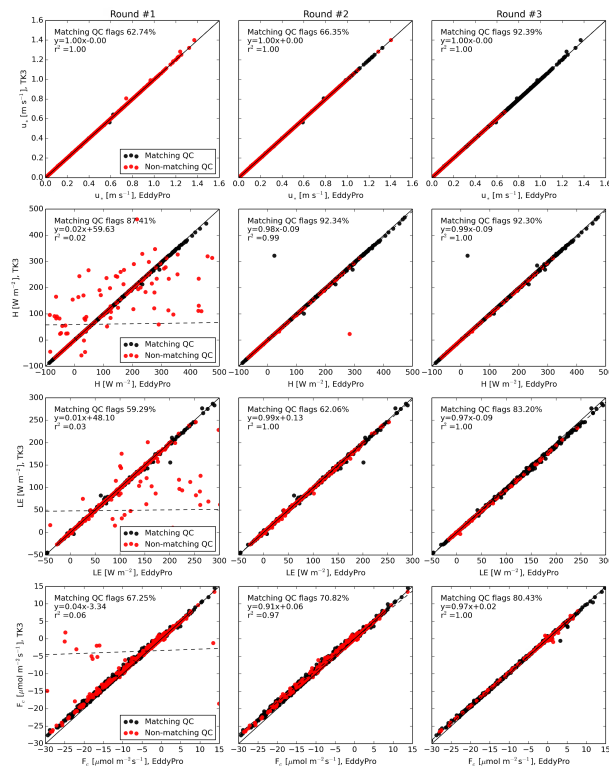


Fig. 1. Scatter plots including regression parameters between friction velocities u_* , sensible heat fluxes H , LE and F_c for the closed-path dataset calculated with EddyPro and TK3. The results of the three comparison rounds with refined software configurations are displayed from left to right. Very poor regression parameters in the first round (leftmost plots) are driven by wildly scattering data points, lying outside the chart areas.

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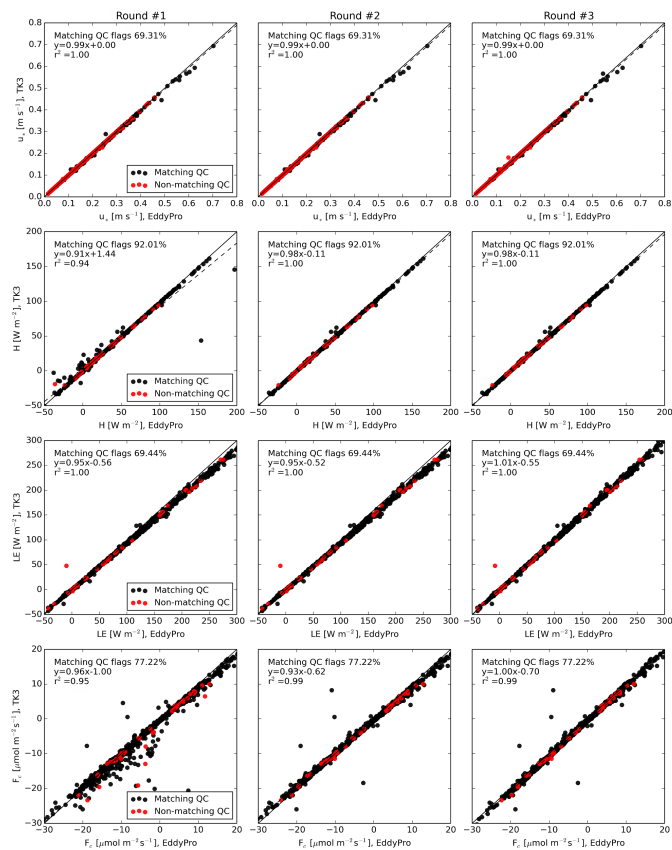


Fig. 2. Same as Fig. 1, but for the open-path dataset.