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V57 QUALITY CONTROL OF VERY SMALL TRACE GAS FLUXES

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1. INTRODUCTION

When measuring turbulent fluxes of trace gases, a threshold value of the friction velocity (u_* threshold) is usually assumed (Goulden et al. 1996) below which fluxes are considered faulty and are replaced according to a gap-filling procedure (Papale 2012). Our measurements in recent years after forest fires (Oliveira et al. 2021), over ice (Jentzsch et al. 2021b), and over permafrost (Jentzsch et al. 2021b; Schaller et al. 2019) surfaces have shown that small fluxes are typical in such environments, and therefore too many measurements would need to be replaced if applying a simple u_*threshold filter. Moreover, common gap-filling algorithms rely on parametrizations of assimilation (Lloyd and Taylor 1994) and respiration (Michaelis and Menten 1913) that may have limited applicability to surfaces that vary widely in terms of their properties like ice or water surfaces.

To improve this situation, we propose a scheme that makes use of all quality flags according to Foken and Wichura (1996) in the data analysis – as already suggested by Ruppert et al. (2006), where a MAD (median absolute deviation) procedure is used to exclude residual false values (Papale et al. 2006). Special attention is paid to flux corrections, which, like the Webb, Pearman and Leuning (WPL) correction (Webb et al. 1980), can be significantly larger in magnitude than the uncorrected fluxes and must be evaluated with an independent flag. Small fluxes are often non-steady state, which can be detected with the above-mentioned flags. The calculation of these small non-steady state fluxes is performed by evaluating the spectra of the wavelet coefficients. Applying this scheme would substantially increase the number of measured values and, thereby, the empirical basis for the determination of the gap-filling procedure.

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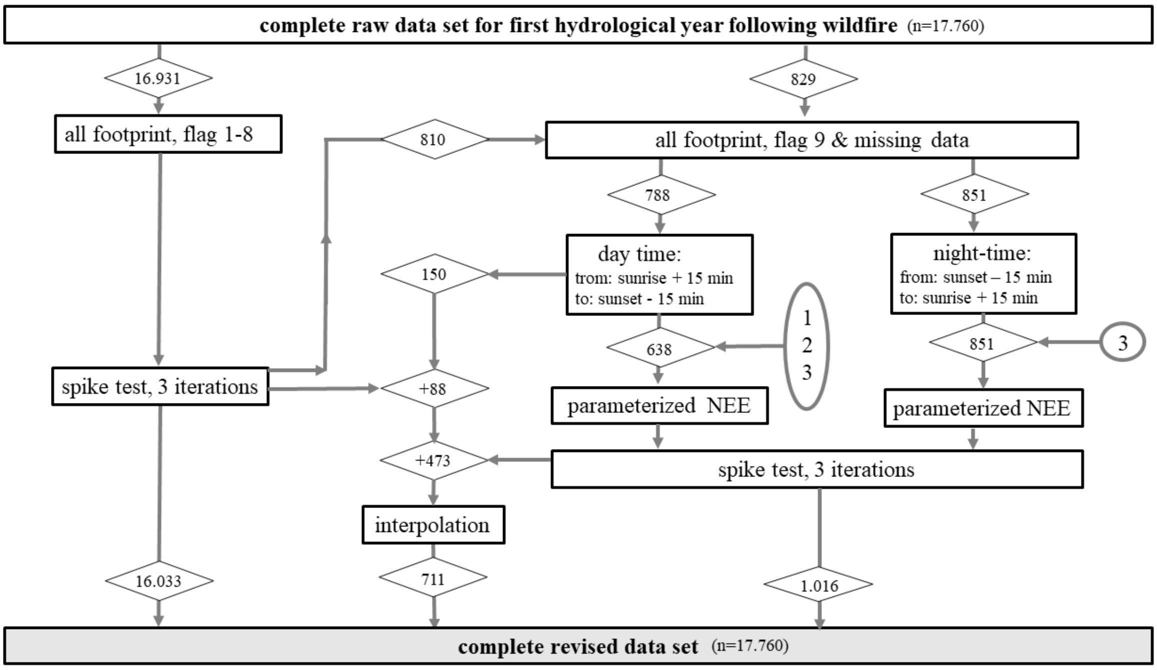

Fig. 1. Flow chart of the revision of the raw data. The numbers indicate the number of half hour data sets at the forest fire site at Vila de Rei, Portugal from 1 October 2017 to 30 September 2018. The jump addresses 1 to 3 refer to the respective gap-filling routines used in the original work (Oliveira et al. 2021, Supplement), © Authors.

2. DATA SETS OF THIS ANALYSIS

Several data sets were used for the present analysis. The development of the evaluation scheme is based on data of the study area (39° 37' N, 08° 60' W) 250 m above sea level located near Vila de Rei, Portugal in a Mediterranean climate zone after a forest fire of the Pine Forest on 13 August 2017. The eddy-covariance system with the sonic anemometer CSAT3 (Campbell Sci.) was located at 11.8 m agl, zero-plane displacement 3.8 m. For details see Oliveira et al. (2021).

The development of the wavelet tool based on observations within the floodplain of the Kolyma River (68.78° N, 161.33° E, 6 m above sea level), situated about 15 km south of the town of Chersky in north-eastern Siberia. The eddy-covariance system with the sonic anemometer uSonic-3 (METEK GmbH) was 4.9 m agl. For details see Kittler et al. (2016).

For the basic investigations of the WPL correction, we used a data set from about 2 km west of the Ny-Ålesund research base on the island of Spitsbergen (78°55′ N and 11°50′ E). The eddy-covariance complex with a CSAT3 (Campbell Sci.) and a LI-7500A open-path infrared gas analyzer (LI-COR Biosciences) was located 2.75 m above the snow-free ground. For details see Jentzsch et al. (2021b). The Portuguese dataset was used for the further investigation.

3. DATA QUALITY CONTROL

Fig. 1 shows the flow chart for processing a one-year data set of the Portuguese site. The basis for the processing was the 10-step flagging system for turbulence data according to Foken and Wichura (1996), which has been published several times in great detail (Foken et al. 2012; Foken et al. 2004; Mauder and Foken 2015), and the footprint analysis according to Kormann and Meixner (2001).

Only the best quality data was used to develop the site-specific gap-filling algorithms. For this purpose, only quality classes 1–3 according to Foken and Wichura (1996) were allowed. Furthermore, 80 % of the measured fluxes had to be assigned to the target surface based on the experience from investigations for European FLUXNET sites (Göckede et al. 2008). The very special gap-filling algorithms for the investigated surfaces are not subject of this investigation, in this respect reference is made to the cited original works.

In order to eliminate some outliers (spikes) from the data selected for parameterization in the gap-filling procedure, the MAD-Test (MAD: Median Absolute Deviation) was applied. The MAD-Test according to Hoaglin et al. (2000), first applied to CO_2 flux data by Papale et al. (2006) and first used for de-spiking raw EC data by Mauder et al. (2013). The MAD-Test identifies as outlier all values that are outside the following range:

$$median(x) - \frac{q\,MAD}{0.6745} < x_i < median(x) + \frac{q\,MAD}{0.6745} \qquad (1)$$

where the factor of 0.6745 stems from the Gaussian distribution, and q is a threshold value that must be determined depending on the specific data set. This spike test was applied multiple times: (i) to the selected dataset for developing the gap-filling algorithms, (ii) to the overall dataset, (iii) to the gap-filled data, where (ii) and (iii) are shown in Fig. 1.

For the data set used for the general evaluation, all data qualities 1–8 according to Foken and Wichura (1996) were used. With respect to the footprint, no restrictions were initially made, but details for individual wind sectors were discussed during the evaluation (Oliveira et al. 2022; Oliveira et al. 2021). Thus, only about 10% of the data needed to be gap-filled. If no gap-filling was possible (spike test), the data were interpolated.

4. WAVELET ANALYSIS

In some of the measurements made after wildfires, over ice and permafrost, different processes are present than those used by conventional gap-filling routines that model assimilation and respiration. Furthermore, for highly non-steady state cases, the flux was determined at 1minute resolution from the spectrum of wavelet coefficients and used for gap-filling. A detailed description of the method is not given here, since it has been published extensively (Schaller et al. 2017) and the basics can be taken from the wavelet literature. Instead, the result shown in Fig. 2 will be discussed below.

The upper graph in Fig. 2 shows the time course over 2 hours of the methane concentration and the vertical wind speed. At least by the course of the concentration the measurement would be marked as non-steady state and would be replaced by a gap-filling procedure. In

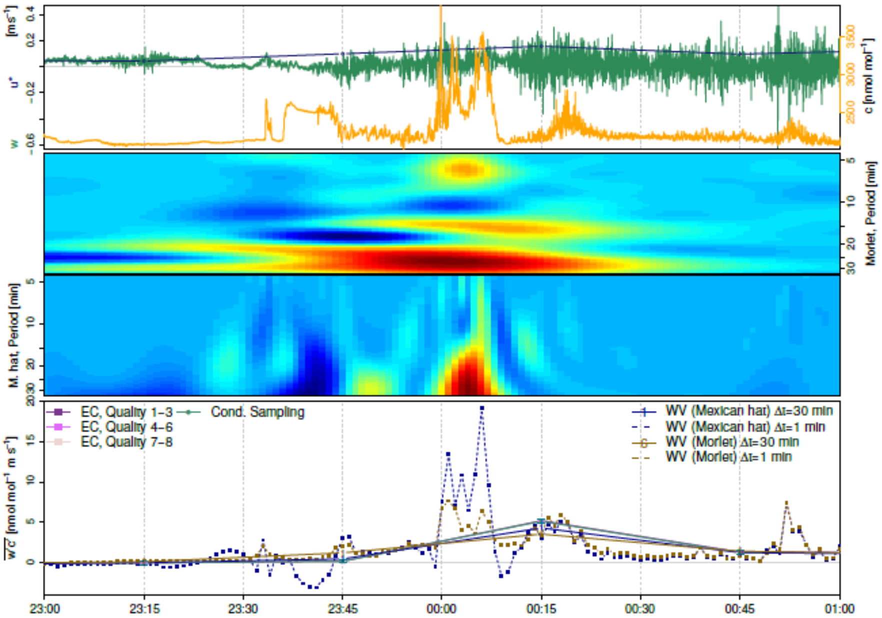

Fig. 2. Case study of 02/03 August 2014. The colours in the wavelet cross-scalograms between w and c denote the flux intensity, blue refer to the smallest, green to medium and red to highest methane flux contributions. Dashed lines represent wavelet fluxes with an averaging period of 1 min. For details see text. (Schaller et al. 2017), © Authors

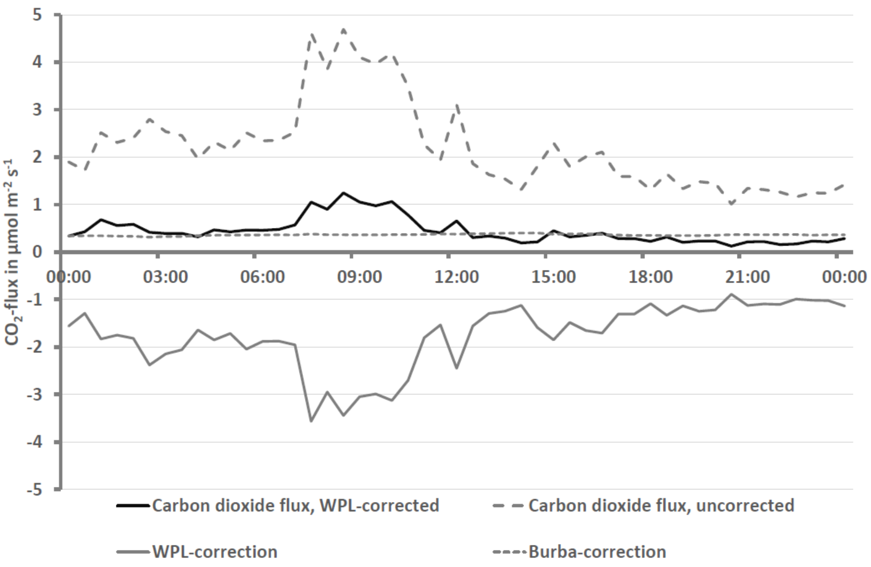

Fig. 3. Comparison of WPL-corrected and uncorrected CO_2-flux together with the size of the WPL- and Burba-correction on 06 December 2015 at the Bayelva site, temperature range 268–270 K. The Burba correction (Burba et al. 2008) that may be relevant for this temperature range is also shown. (Jentzsch et al. 2021a), © Authors

the middle part of the graph two wavelets are shown, the Morlet wavelet with a good frequency characteristic and the Mexican Hat wavelet with a good temporal characteristic, the latter being able to represent the i non-steady state conditions well. In the lower graph, the fluxes determined with both wavelets are calculated with 1minute resolution. Furthermore, the averaging over 30 minutes is shown in comparison to the classical eddy-covariance evaluation. The Mexican Hat wavelet can represent the non-steady state flux well and forces larger fluxes over 30 minutes than the classical calculation. The tool can thus be used for gap-filling non-steady state measurements.

5. WPL-CORRECTION

Most of the necessary corrections of the eddy-covariance method for determining turbulent fluxes are relative corrections, i.e., for small fluxes these corrections also remain small and do not significantly modify the measurements. However, the density correction according to Webb et al. (1980) is an additive correction. It is often significantly larger than the measured flux, and the correction modifies the flux significantly including a possible correction for sign (Fig. 3). A test has been developed that relates the correction to the corrected flux (Jentzsch et al. 2021a). A possible quality flag could be the ratio of WPL correction and corrected trace gas flux:

$$QF_{WPL} = \frac{\{\text{WPL}-\text{correction}\}}{\{\text{measured flux}\}+\{\text{WPL}-\text{correction}\}} \quad (2)$$

If the correction is only 10% of the corrected flux, high quality was assumed, in the 5-year Vila de Rei data set in about 35% of the cases (Fig. 4). If the correction exceeded the corrected flux by a factor of 5, the data were discarded. However, setting the limits for the quality flag requires further investigation with other data sets.

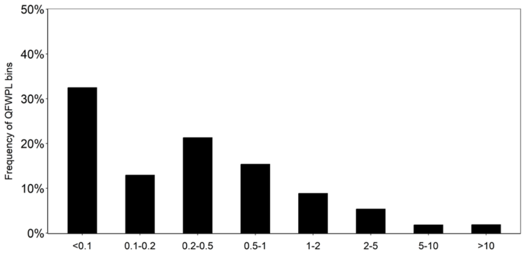

Fig. 4. Frequency of WPL quality flag according to Eq. (2) from 26 September 2017 to 30 September 2022 for the Vila de Rei, Portugal, data set. © Bruna R. F. Oliveira

6. CONCLUSIONS

The proposed scheme requires some manual and programming effort, also standard programs can be used for eddy-covariance evaluation. However, the data processing schemes of measurement programs such as ICOS (Sabbatini et al. 2018) do not contain all the necessary data that must be calculated subsequently. Especially when measuring relatively small fluxes, one should make the increased effort, at least for process studies.

Applying this scheme would substantially increase the number of measured values and, thereby, the empirical basis for the determination of the gap-filling procedure. For the 1-year data set of the Villa de Rei site 2017/2018 (Fig. 1), the number of measured values still to be replaced by gap-filling after application of the procedure would be reduced from 50 % (classical u_* threshold) to approx. 10 %. One advantage of the proposed procedure is that it does not lead to a bias towards higher fluxes which is transferred to accumulated fluxes.

The calculation of fluxes with the wavelet tool should be applied for very non-steady state fluxes and for gap-filling of trace gas fluxes, where the standard routines for assimilation and respiration cannot be applied. However, the year-round calculation of methane fluxes with the tool and with the standard 30-minute calculation showed no meaningful differences in the cumulative fluxes (Göckede et al. 2019).

The additional quality flag for WPL correction for small fluxes certainly seems reasonable after further testing and should be implemented in the eddy-covariance standard software.

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