



JGR Biogeosciences

Supporting Information for

Atmospheric CO₂ exchange of a small mountain lake: limitations of eddy covariance and boundary layer modeling methods in complex terrain.

Katharina Scholz^{1*}, Elisabet Ejarque², Albin Hammerle¹, Martin Kainz², Jakob Schelker^{2,3},
Georg Wohlfahrt¹

- 1) Department of Ecology, University of Innsbruck, Sternwartestrasse 15, 6020 Innsbruck, Austria.
- 2) WasserCluster Lunz – Biologische Station, Dr. Carl Kupelwieser Promenade 5, 3293 Lunz am See, Austria.
- 3) Department of Functional and Evolutionary Ecology, University of Vienna, Althanstrasse 14, 1090 Vienna, Austria.

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Introduction

Because the ogive optimization (OgO) method is not commonly applied in eddy covariance (EC) data processing, a short summary of the method and its background as developed and described by Sievers et al. (2015 a) is given in the following. In addition, the application of the OgO method at our field site – a small mountain lake – is exemplified and discrepancies between the estimated fluxes resulting from the OgO method and the conventional EC data processing are presented.

Text S1 – Additional information on the ogive optimization method.

The OgO is an alternative approach to process EC data to estimate turbulent exchange while separating out low-frequency contributions (Sievers et al., 2015).

An ogive is an empirical cumulative distribution and here refers to the cumulative integral of the co-spectra of CO₂ concentration and vertical wind speed (w) from high to low frequencies, where the co-spectrum is the spectral decomposition of the flux estimate. Therefore, an ogive represents the cumulative contribution of different frequencies to the calculated flux. In theory, the ogive converges towards an asymptote with decreasing frequencies within an optimum averaging interval (Figure S1 a). However, the inclusion of low frequency contributions may lead to a continuous increase (Figure S1 b) or reversal (Figure S1 c) of the ogive curve depending on the direction of the low frequency motions. Low frequency contribution can be minimized by choosing the ideal averaging interval. Also, pre-treatment of the data with an appropriate detrending method can help to reduce non-turbulent influence. However, in cases where the frequency range of turbulence and low-frequency contributions overlaps, the estimation of the ideal averaging time or detrending method is not straightforward.

The OgO method generates an ogive density map by calculating ogives for a multiplicity of data permutations based on different combinations of averaging times and detrending methods for a certain time window at any chosen point in time (Figure S1, grey shades). Subsequently, a spectral distribution model is fitted to the obtained density map and the best fit (Figure S1, blue lines) is assumed to represent the pure turbulent flux.

In our study, the EC method was used to quantify lake-atmosphere CO₂ exchange. Fluxes calculated using the standard EC processing (using EddyPro 6.2.1, LI-COR Inc., Lincoln, NE, USA) showed large short-term temporal variation and the spectral analysis of the raw data indicated high low-frequency contributions. Therefore, the OgO method was applied to calculate CO₂ fluxes (F_{c-Og}) at this small mountain lake and the results were compared to the flux results of the standard EC processing (F_{c-EC}). In addition, the prevailing environmental conditions in relation to the differences between the results of the two processing methods were analyzed. To that end, a regression ensemble was trained to predict the differential CO₂ flux between the two processing methods based on air temperature (T_a), the surface water temperature estimated from outgoing longwave radiation (T_s), relative humidity (RH), net solar radiation (R_n), wind speed (u), friction velocity (u^*), atmospheric stability (z_{oL}), and wind direction at the opposing shore (u_{dir_w}) and the predictor importance and the related partial dependence were investigated. All analyzes were done in Matlab version R2019b (The MathWorks Inc., Natick, MA, USA).

In Figure S1, three examples for OgO flux estimations at Lake Lunz are shown. In all three panels, the red line marks the ogive as calculated for a 30min averaging interval with data linearly detrended, i.e., the conventional EC processing. The grey shades show the ogive density map based on the respective data permutations while the resulting modeled ogive is represented by the blue line. Panel a) shows a case where the conventionally calculated ogive

(red line) closely follows the expected shape converging towards a constant value (about $0.4 \mu\text{mol m}^{-2} \text{s}^{-1}$ in that case) at the low frequency range (left end of the x axis). Therefore, the difference between $F_{\text{c-EC}}$ and $F_{\text{c-Og}}$ is small. However, at Lake Lunz, cases as depicted in panel b) and c) were more common, with variable low-frequency contributions often causing an unexpected increase or reversal of the ogive curve.

Overall, fluxes calculated using the OgO method showed less scatter than the conventional processing (Figure S2) and also a better agreement with the seasonal course of dissolved CO_2 and CO_2 flux estimates based on the BLM method, $F_{\text{c-BLM}}$ (Figure S3).

The best predictors for differences in the fluxes calculated with the two processing methods ($F_{\text{c-EC}}$ and $F_{\text{c-Og}}$) were wind speed and the wind direction at the opposing shore (which is an indicator of the persisting wind regime) (Figure S4 upper panel). In general, low wind speed and lake-breeze conditions led to the largest discrepancies between the two flux estimates (Figure S4 lower panels).

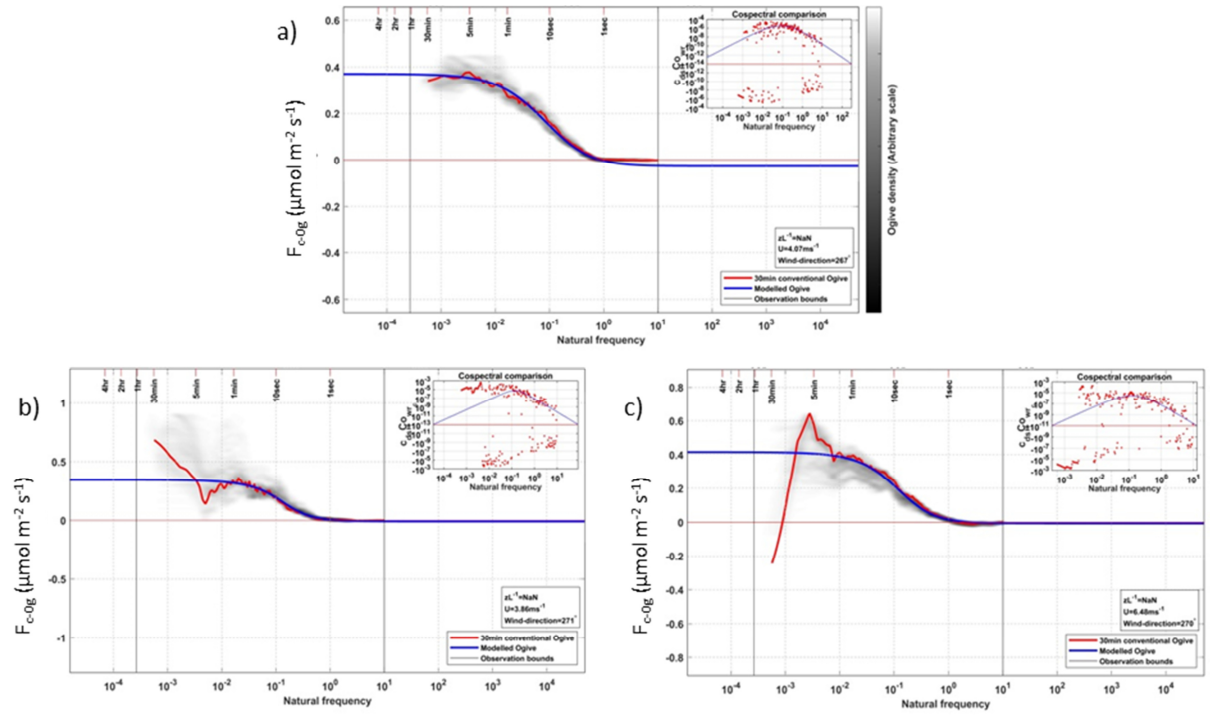


Figure S1. Three exemplary cases for flux estimates using the OgO method. The red line shows the standard 30min linear detrending. The grey shades denote the ogive density pattern of ogives calculated following data permutations. The best fit modeled ogive is shown in blue. The small inserted figures show equivalent co-spectra. Three situations are shown, where a) the standard ogive closely follows the expected shape and discrepancies between standard and modeled ogive are small, b) low-frequency contributions lead to a continuous increase of the ogive curve and therefore to flux overestimation, and c) low-frequency contributions cause a sign reversal and therefore to flux underestimation.

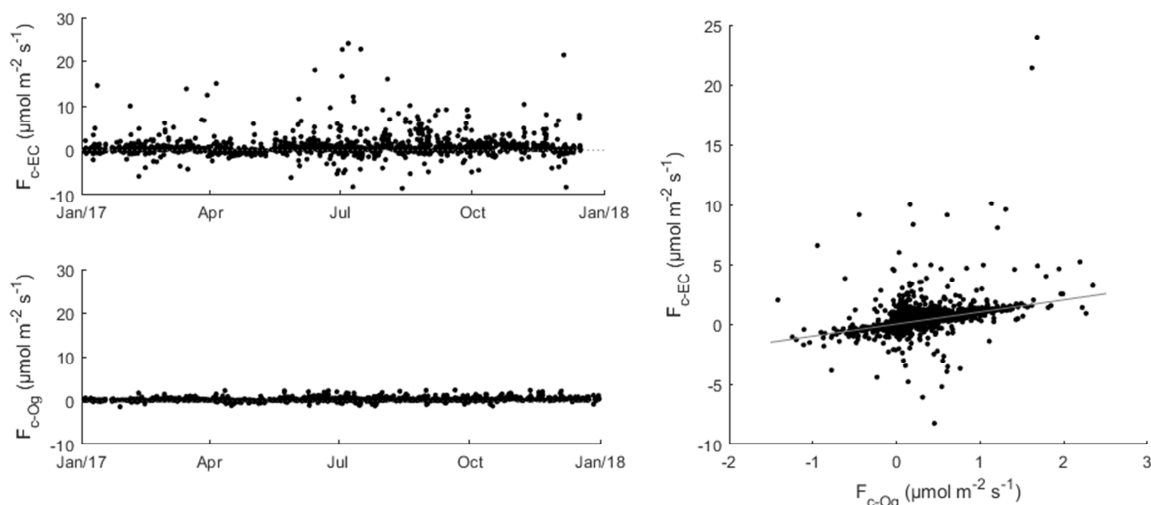


Figure S2. CO₂ flux estimates based on the standard EC processing (F_{c-EC} , top left), based on the OgO method (F_{c-Og} , bottom left), and a scatter plot of F_{c-EC} and F_{c-Og} . The grey line in the scatter plot denotes the 1:1-line.

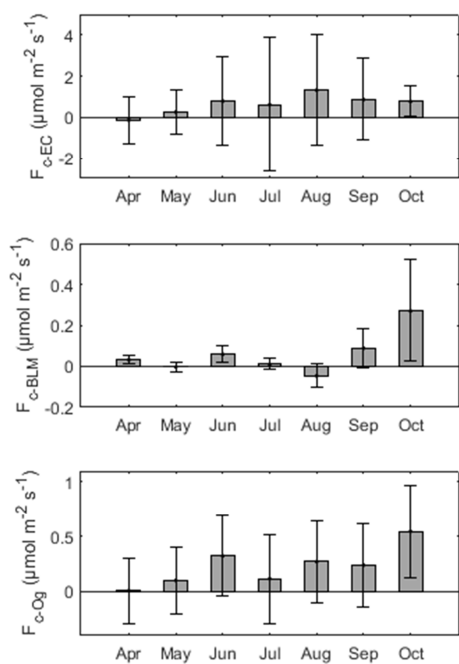


Figure S3. Monthly mean CO₂ fluxes estimated based on the standard EC (top), the BLM (middle), and the OgO (bottom) approach. Error bars show ± 1 standard deviation.

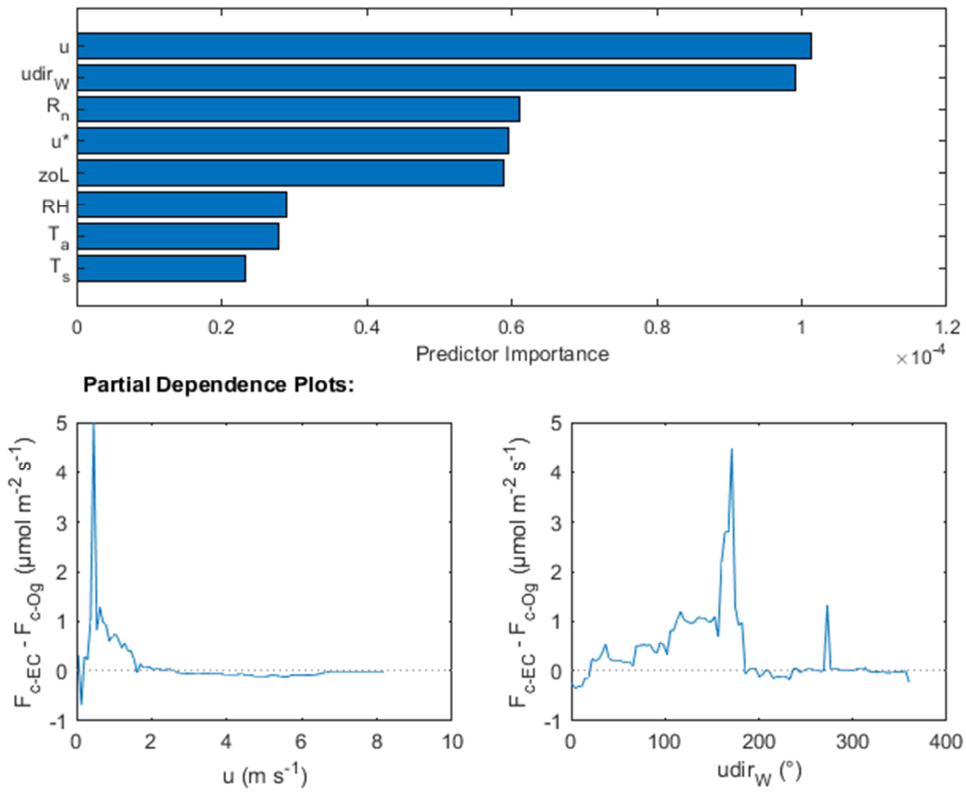


Figure S4. Predictor importance (top panel) of the trained regression ensemble. The partial dependence of the two most important predictors, wind speed u and wind direction at the opposing shore $udir_w$, is plotted in the lower panels.

Table S1. Overview of EC CO₂ flux measurements at lakes – additional information.