

Original Software Publication

fluxfixer: An R package for producing thermal dissipation sap flow data with high quality control

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ABSTRACT

The thermal dissipation method is crucial for estimating tree transpiration, a major component of terrestrial water cycling. However, this method requires careful quality control (QC), and no post-processing software exists for automatic QC that can apply to raw time series with various artifacts. Hence, we developed a novel R package to conduct sophisticated QC combined with statistical methods and machine learning. We further provided selective methods for calibrating the zero-flow conditions. We demonstrate the package's effectiveness by post-processing raw data observed in a Bornean tropical rainforest. This package will help establish a standardized protocol for processing low-quality sap flow data.

Metadata

Nr	Code metadata description	Metadata
C1	Current code version	V1.1.0
C2	Permanent link to code/repository used for this code version	https://CRAN.R-project.org/package=fluxfixer and https://github.com/yhata86/fluxfixer
C3	Permanent link to reproducible capsule	None
C4	Legal code license	MIT + file LICENSE
C5	Code versioning system used	Git
C6	Software code languages, tools, and services used	R
C7	Compilation requirements, operating environments, and dependencies	R ≥ 4.0 and R packages: dplyr, gsignal, lubridate, magrittr, ranger, rlang, stats, tidyr, tidyselect, xts, zoo
C8	If available, link to developer documentation/manual	https://yhata86.github.io/fluxfixer/
C9	Support email for questions	yoshiakihata0806@gmail.com

1. Motivation and significance

Plant transpiration is among the most essential components in the terrestrial water budget. Globally, approximately two-thirds of total precipitation over land returns to the atmosphere through terrestrial

evapotranspiration [1]. Global-scale studies using various methods, including isotope, modelling, site-measurement, and remote-sensing approaches, have shown that plant transpiration accounts for nearly sixty percent of terrestrial evapotranspiration [2–6]. Thus, the vegetation transpiration plays a key role in the Earth's water cycle and regulates ecosystem water resource availability. However, transpiration changes according to the environmental conditions and is affected by complicated non-linear feedback [7], causing considerable uncertainty in future transpiration and water cycling projections [8]. Therefore, accurately measuring *in-situ* transpiration during ongoing climate change is crucial for reducing uncertainty.

Heat tracer-based sap flow measurements have been widely used for estimating plant transpiration because of their ease of implementation, replication, and automation [9]. One common type of tree sap flow sensor is the thermal dissipation method (TDM) probe developed by Granier [10,11] because it is relatively simple and economically efficient [12,13]. TDM measures the temperature difference (ΔT ; °C) between a heated and reference sensor. Given the maximum temperature difference between the probes when sap flux is assumed to be zero (ΔT_{\max} ; °C), ΔT can be converted into sap flux density (F_d ; $\text{m}^3 \text{m}^{-2} \text{s}^{-1}$) using the following equation:

$$F_d = \alpha K^\beta \quad (1)$$

where

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$$K = \frac{\Delta T_{\max} - \Delta T}{\Delta T} \quad (2)$$

Here, K is a dimensionless index and α and β are empirical parameters [10,11]. To accurately estimate F_d , high-quality ΔT time series must be observed. However, unstable power, insufficient probe insertion, probe degradation, and sapwood wounding effects often make the ΔT time series noisy and non-stationary [12,14,15]. Fig. 1 shows typical artifacts in observed time series, demonstrating the necessity of careful data quality control (QC).

Several software packages provide QC protocols and post-processing for sap flow data [14,16–18]. However, their protocols are difficult to apply to long-term noisy data, especially for outlier detection and gap filling. This is because they use statistical methods to analyze the time series of the original variables and/or differential variables between two time points and remove points whose statistical values exceed certain

thresholds. These methods are good at identifying out-of-range values and spikes, but ineffective for determining unreasonable in-range values or sequential outliers. Moreover, visual inspection for outlier detection is allowed, introducing subjectivity into the analysis. To fill gaps, they provide interpolation such as spline fitting, which is only reasonable for short-term data gaps. Because transpiration is affected by meteorological and soil conditions, longer data gaps can only be reasonably filled by considering such physical environment information.

Here, we present *fluxfixer*, a novel software that enables users to conduct QC and output continuous sap flow time series using statistical methods and machine learning. This package can help researchers who have noisy sap flow data that are difficult to handle, facilitating the publication of substantial sap flux datasets.

Ideally observed time series

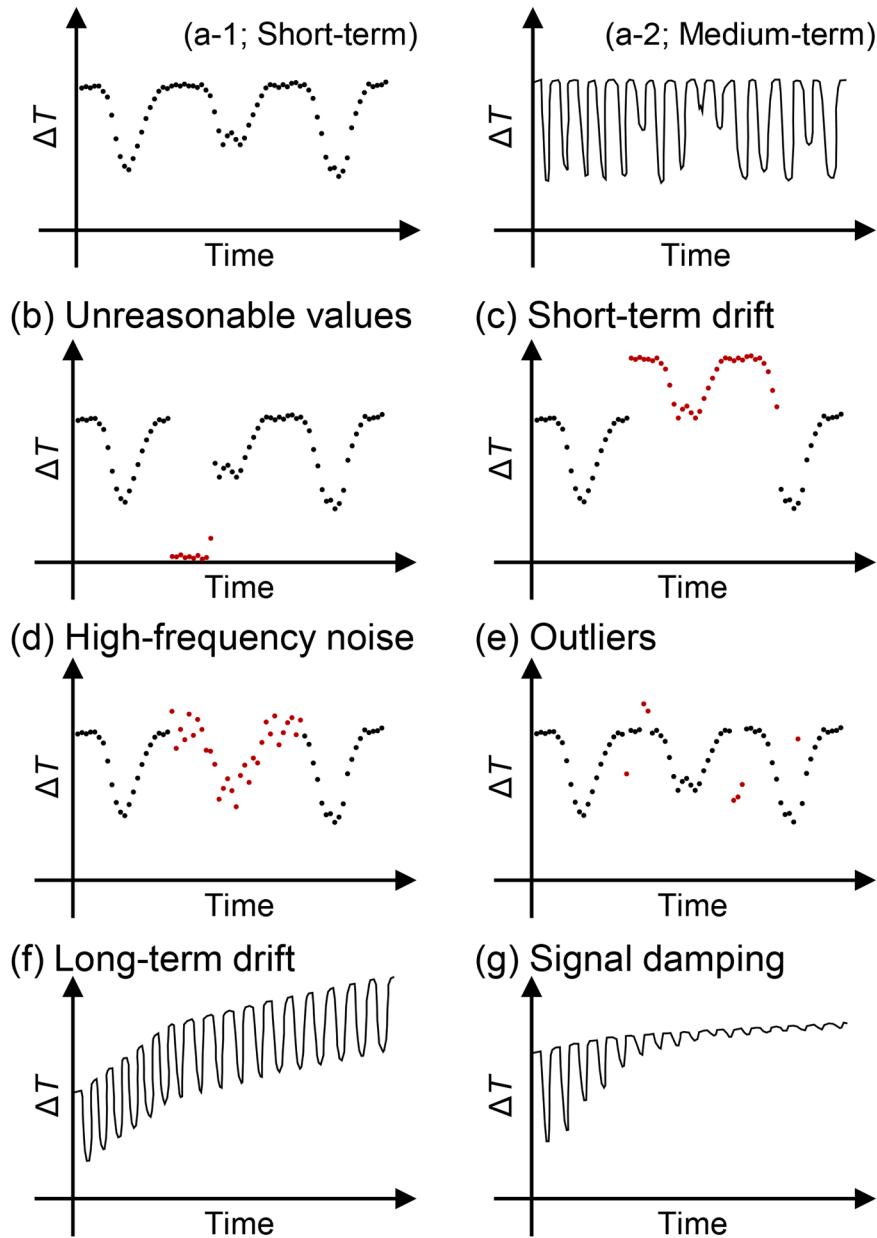


Fig. 1. Examples of probe temperature difference (ΔT) time series: ideal observed series for (a-1) short-term and (a-2) medium-term periods, (b) unreasonable values due to power supply interruption, (c) short-term drift, (d) high-frequency noise contamination, (e) outliers in and outside the reasonable range, (f) long-term drift, (g) and signal damping. Unreliable data points are shown in red.

2. Software description

The fluxfixer open-source software package is written in the R language [19], and includes step-by-step functionality as well as one that conducts all processes automatically. fluxfixer works in a command-line interface without a graphical user interface. Hence, users can record all the commands used in data processing into a single text file, ensuring reproducibility.

2.1. Software architecture

Fig. 2 presents the developed software’s architecture. First, users prepare an input dataset that includes the time-stamped raw ΔT time series. Then, anomaly correction and outlier removal are applied to the input ΔT time series. After the data cleaning, gaps are filled by a machine-learning model to make the time series continuous. Using this time series, the ΔT_{\max} time series is calculated by various methods. Finally, F_d is calculated using Eqs. (1) and (2), and users can obtain the computed time series of ΔT , ΔT_{\max} , F_d , and QC flag. Each step is further explained as follows.

2.1.1. Data input

The input dataset must include evenly spaced time stamps in local time and the corresponding ΔT time series. Any time step is acceptable, but we assume the typical time step is less than one hour. Meteorological, soil environment, and ecophysiological factor time series can also be included. Although not mandatory, we highly recommend including a time series for vapor pressure deficit because it typically regulates stomatal opening [20]. If the sap flow measurement is conducted in forests with high seasonality, such as deciduous forests, we recommend including a time series for the amount of forest leaf, e.g., the leaf area index.

2.1.2. Anomaly correction

The first step in the process is to remove anomalies and correct the time series. This step is divided into three procedures: (1) The absolute limit test specifies the range of valid ΔT values and removes points that deviate from that range. The thresholds in the function can be defined as any value, but a $\Delta T < 3 \text{ }^\circ\text{C}$ or $> 50 \text{ }^\circ\text{C}$ is considered an anomaly by default. (2) The short-term drift correction is an optional method to correct sudden changes in the average in the time series over a user-selected short period (hours to days). This procedure uses a reference period, which is defined to consist of the three days before and after the occurrence of the anomaly by default. Then, the anomalous time series is standardized so that the 5th and 95th percentile values of the anomalous and reference (non-anomalous) time series match over this period. That

is,

$$x_{\text{corrected}} = \frac{x_{\text{raw}} - x_{\text{raw}}^{5\text{th}}}{x_{\text{raw}}^{95\text{th}} - x_{\text{raw}}^{5\text{th}}} (x_{\text{ref}}^{95\text{th}} - x_{\text{ref}}^{5\text{th}}) + x_{\text{ref}}^{5\text{th}} \quad (3)$$

where $x_{\text{corrected}}$, x_{raw} , and x_{ref} are the corrected, original, and reference x variables, respectively. The superscripts “95th” and “5th” respectively indicate the 95th and 5th percentiles of the specific time series. These values are used rather than the maximum and minimum values to ensure robustness to possible outliers in the original or reference time series. (3) High-frequency noise removal is an optional step that is applied when the observed time series is contaminated with high-frequency noise. Users obtain a low pass-filtered time series by convolving it with a Gaussian window function over a user-selected period.

2.1.3. Outlier removal

The outlier removal process is performed as follows: (1) The entire time series is normalized using a moving window, and the data values are converted to Z-scores. In this step, the width of the moving window is set to 15 days by default and is centered on the target time point, and normalization is performed individually for all time points in the time series. The upper and lower limits of the Z-score (default $Z = \pm 5$) are set, and data points outside that range are removed as outliers. After the outliers have been removed, the Z-score is returned to the original value using the original mean and standard deviation time series, and normalization is performed again using a moving window to remove additional outliers. These procedures are repeated until either no more outliers are removed or the maximum number of iterations (default 10) is reached.

(2) A random forest, which is a machine-learning model, is constructed for the stationary Z-score time series. The user can input any feature from the dataset, and out-of-bag evaluation is used to determine the hyperparameters. To reduce the computational cost, the only hyperparameter used by default for grid search is the number of candidate features. To reduce the risk of learning noise, the training data sampling ratio is set to be 0.1 by default. After determining the optimal hyperparameters, they are used to construct the optimal random-forest model. Output values are obtained from 500 (default) trees, and the first quartile (Q1), third quartile (Q3), and interquartile range (IQR) of the output values at each time point are calculated. If the observed Z-score value is less than $Q1 - 1.5IQR$ or more than $Q3 + 1.5IQR$, the data point is identified as an outlier and removed.

In some cases, the ΔT time series may yield a signal that is attenuated for only a short period, for example, when rainfall continues for days, causing the moving window mean (or standard deviation) to increase (or decrease). In such cases, normalization will cause the Z-score time

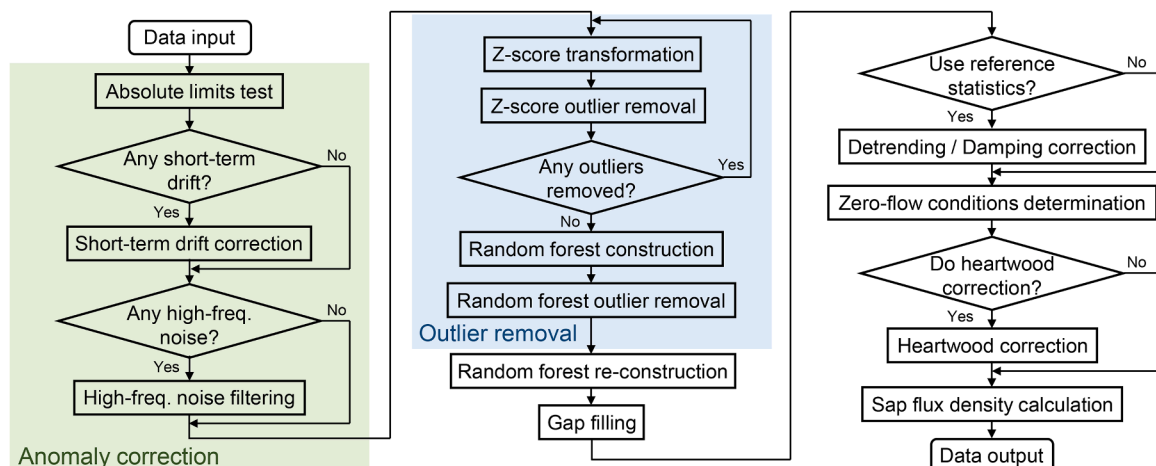


Fig. 2. Data processing in the fluxfixer package. The anomaly correction and outlier removal procedures are shaded in green and blue, respectively.

series immediately before and after the rainfall to be unnaturally distorted, hindering the construction of the random-forest model. For this reason, this function has an optional argument that corrects the Z-score when the signal attenuates for a short period. In addition, although we do not recommend outlier removal by visual inspection because of its high subjectivity, we provide an optional function for manual outlier removal for those who wish to use it.

2.1.4. Gap filling

In this step, all missing values are filled using a random-forest model. Note that the target of missing value imputation is the time series converted to the Z-score, not the original ΔT time series. As in the outlier removal step, the optimal hyperparameters are determined, and a new random-forest model for filling gaps is constructed. We recommend using the physical environment and ecophysiological factors in the dataset as input features to reflect their effects on sap flow dynamics. The model's predicted values are then used for imputation.

2.1.5. ΔT time series retrieval

Once a continuous Z-score time series has been obtained, the Z-score values are converted to ΔT values using the mean and standard deviation time series calculated using the original ΔT time series. Optionally, the Z-score can be converted to ΔT using the mean and/or standard deviation of the time series over 15 days (default) after sensor insertion as a reference value. If the reference mean is used for the conversion, the time series can be detrended, and if the reference standard deviation is used for the conversion, the time series can be corrected for signal damping. In other words, users can correct for long-term trends and signal damping simultaneously.

2.1.6. Zero-flow conditions determination

The daily ΔT_{\max} time series is calculated using the quality-controlled ΔT time series. Users can select any combination of four existing methods, the predawn (PD), maximum moving window (MW), double regression (DR), or environmental dependent (ED) methods [12,14,15], or the successive predawn (SP) method, which is proposed in this study. The SP method defines the ΔT_{\max} for a day as the maximum ΔT within a 24-hour period that begins at 5:00 a.m. (default; just before daybreak in temperate zones). In other words, the day starts at predawn, not midnight, and the maximum value for that period is assumed to be ΔT_{\max} . This method has the advantage of being able to calculate ΔT_{\max} quickly while minimizing the effect of nocturnal transpiration on ΔT_{\max} estimation.

2.1.7. Sap flux density calculation

After determining the zero-flow conditions, F_d is calculated using Eqs. (1) and (2). If the sapwood width is shorter than the probe insertion length, ΔT can be overestimated, leading to the underestimation of F_d . Therefore, heartwood correction is required to correct ΔT [21]. Optionally, before calculating F_d , users can replace ΔT with the corrected ΔT (ΔT_{sw}) by specifying the ratio of the probe length to sapwood width (γ) as follows:

$$\Delta T_{sw} = \frac{\Delta T - (1 - \gamma)\Delta T_{\max}}{\gamma} \quad (4)$$

2.1.8. Data output

Users can obtain the continuous time series of ΔT , ΔT_{\max} , F_d , and the QC flag, which has the same number of time steps as the input time series. Users can use the QC flag time series to distinguish between the original, corrected, and gap-filled values.

2.2. Software functionalities

Table 1 presents an overview of the major functions in fluxfixer. Details for each function are available on the help page in the package.

Table 1

Major functions in the fluxfixer R package.

Function name	Description
run_fluxfixer	Run all processes automatically
check_absolute_limits	Perform the absolute limits test
modify_short_drift	Correct short-term drift
filter_highfreq_noise	Filter high-frequency noise
remove_zscore_outlier	Remove outliers using the Z-score method
remove_rf_outlier	Remove outliers using a random-forest model
fill_gaps	Fill in missing values using a random-forest model
calc_dtmax	Estimate the ΔT_{\max} time series using the selected methods
calc_fd	Calculate the sap flux density including heartwood correction

One advantage of the functions in fluxfixer is that they allow users to perform highly flexible processing by providing access to the internal process through a wide range of arguments. For example, the thresholds for removing outliers as well as the parameters in Eqs. (1) and (4) can all be changed through arguments. This high level of flexibility will facilitate QC optimization for the observed data of various vegetations.

3. Illustrative example

Here, we demonstrate the processing of raw sap flow data measured in a Bornean tropical rainforest from 2012 to 2017. The sap flow measurement was carried out in a natural forest (4°12'N, 114°02'E; 200 m a.s.l.) in the Lambir Hills National Park, located in the northern coastal area of Borneo, Malaysia. Mean annual rainfall and air temperature at the study site from 2010 to 2019 were approximately 2751 mm and 26.2 °C, respectively, with limited seasonal variations [22,23]. The mean canopy height and leaf area index at the study site were approximately 40 m and 6.2 m² m⁻², respectively [24]. We set three measurement plots (484 m² in total area) in the study site, and TDM sensors were inserted into all trunks whose diameter at breast height was >10 cm.

Fig. 3a shows an example of the half-hourly raw ΔT time series observed from *Dryobalanops aromatica* at depths of 0–20 mm. The time series was quite noisy and unstable, mainly owing to power supply instability. A short-term drift can be seen in 2013. Moreover, the time series trend changed when the sensor was replaced, and signal damping occurred from June 2015 to February 2016. First, anomaly correction was performed (Fig. 3b). The absolute limits test removed the values observed during the power shortages, and short-term drift correction removed the drastic increase in values after power was restored. High-frequency noise filtering was not required for this time series.

Next, the ΔT time series was converted into Z-scores for outlier removal (Fig. 3c). The long-term changes in the average value and standard deviation of the original time series were corrected by conversion using a moving window. In this outlier detection step, we removed eight data points whose Z-scores were less than the threshold value. To remove more potential outliers, we constructed a random-forest model with the following input features: half-hourly data for precipitation, solar radiation, vapor pressure deficit, air temperature, wind speed, volumetric soil water content, and the time of day (Fig. 3d). The random forest captured the diurnal cycles of the Z-score time series and identified outliers that deviated from the predicted behavior. We constructed another random forest using the same input features to fill the gaps (Fig. 3e). We retrieved the ΔT time series using the reference ΔT average and standard deviation to conduct detrending and signal damping correction. The retrieved ΔT time series has the stationary characteristics shown in Fig. 3f. This example shows how effectively this software can convert the disordered ΔT time series in Fig. 3a into the clean time series in Fig. 3f. After obtaining the continuous ΔT time series, we determined the zero-flow conditions. Fig. 3g, h show an example of estimating ΔT_{\max} and F_d , respectively, using the SP, PD, and MW methods, which use a similar approach to determine ΔT_{\max} . The PD method does not consider nocturnal transpiration, leading to relatively

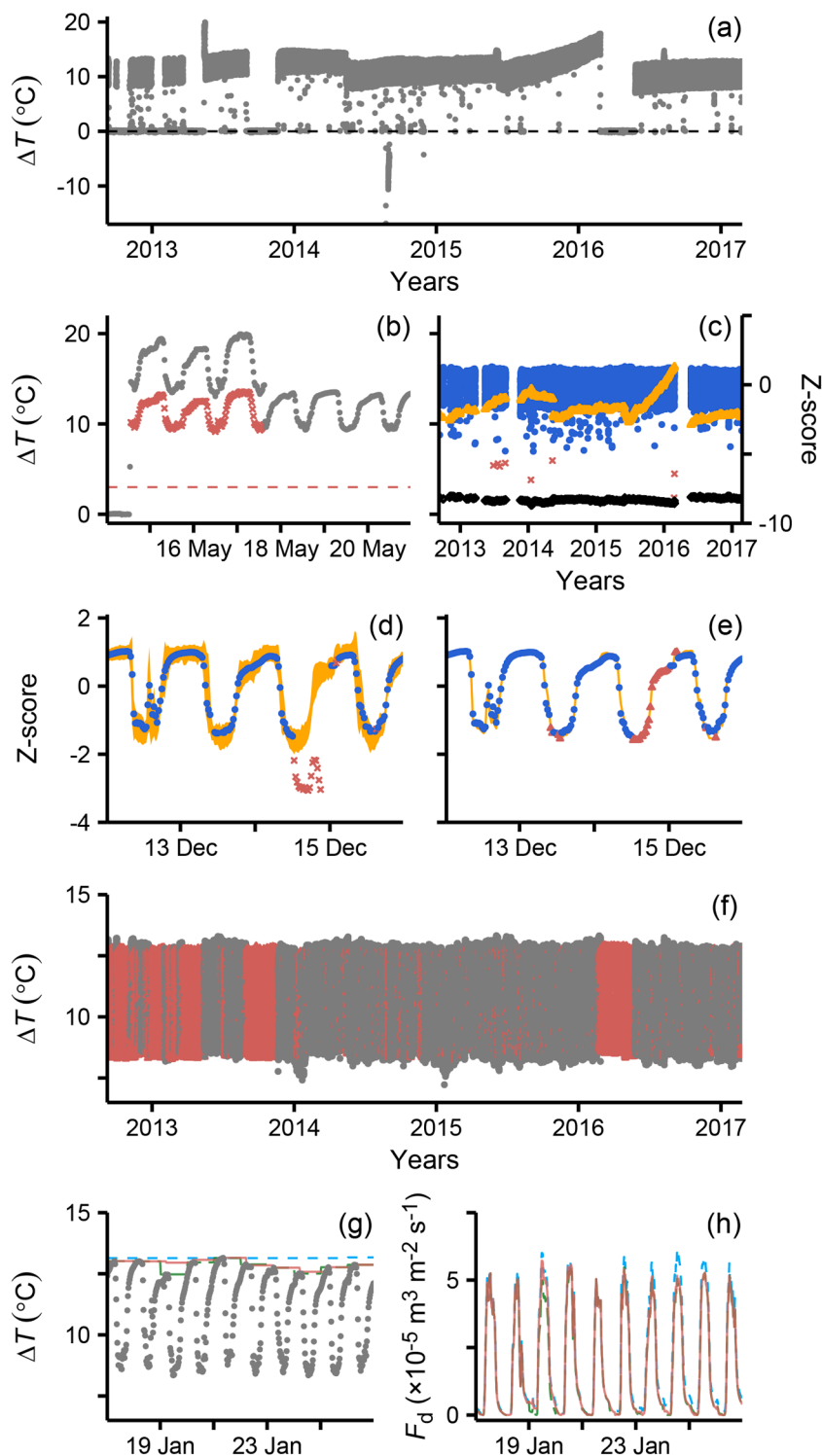


Fig. 3. Examples of the target time series after major steps in the fluxfixer package. All points in the figure represent half-hourly data values. (a) Raw probe temperature difference (ΔT) time series over the whole observation period. (b) ΔT time series after anomaly correction (14–20 May 2013). The dashed line indicates the threshold for the absolute limits test. Raw and corrected values are depicted as gray circles and red crosses, respectively. (c) Z-score time series after Z-score outlier removal (blue circles). The Z-score points detected as outliers are depicted as red crosses. Moving window average (°C) and standard deviation (°C) time series are shown as orange triangles and black diamonds, respectively. (d) Z-score time series after outlier detection by the random-forest model (12–15 December 2016). Blue circles and red crosses represent reasonable Z-score values and detected outliers, respectively. The orange zone indicates the acceptable range estimated by the model. (e) Gap-filled Z-score time series over the same period as that of (d). Original and gap-filled values are indicated by blue circles and red triangles, respectively. The orange line represents the values estimated by the random-forest model. (f) Gap-filled ΔT time series. Non-gap-filled and gap-filled data points are indicated by gray circles and red triangles, respectively. (g) Gap-filled ΔT (gray circles) and the maximum probe temperature difference (ΔT_{max}) time series calculated by the SP (red line), PD (green line), and MW (blue line) methods (17–26 January 2016). (h) Continuous sap flux density (F_d) time series calculated using the SP (red line), PD (green line), and MW (blue line) methods over the same period as that of (g).

lower F_d on the following day. The MW method may not capture a decrease in ΔT_{\max} over several days, leading to relatively higher F_d . Despite a need for further verification, the SP method appears to have the potential to estimate ΔT_{\max} by effectively distinguishing singular and several-day decreases in nighttime ΔT . Note that when we input only mandatory variables (time stamps and ΔT) to the function, filling long-term gaps failed to reproduce the ΔT and F_d daily variation (Fig. 4a, b), highlighting the importance of inputting various variables affecting ΔT .

4. Impact

Sap flow measurements using the TDM have been conducted globally, and the unified database SAPFLUXNET is becoming more widely used [13,24]. However, SAPFLUXNET still contains few data from

remote tropical regions with a large amount of precipitation, such as natural tropical rainforests [24]. Because the TDM requires continuous heat emission, its raw data often become noisy when the measurements are made using an unstable power supply. Thus, obtaining high-quality raw TDM measurement data from tropical rainforests can be difficult, possibly preventing these data from being published. If data from such areas can be made public using fluxfixer, a global understanding of tree water use is expected to advance.

Additionally, the interpolation or simple empirical models used in previous software are not suitable for filling medium- to long-term gaps, making it impossible to calculate monthly and yearly accumulated values. fluxfixer enables more accurate medium- to long-term gap filling, contributing to further discussions of the seasonal and interannual variations in sap flux and the environmental response of vegetation. Furthermore, this software's outlier removal method can be applied not

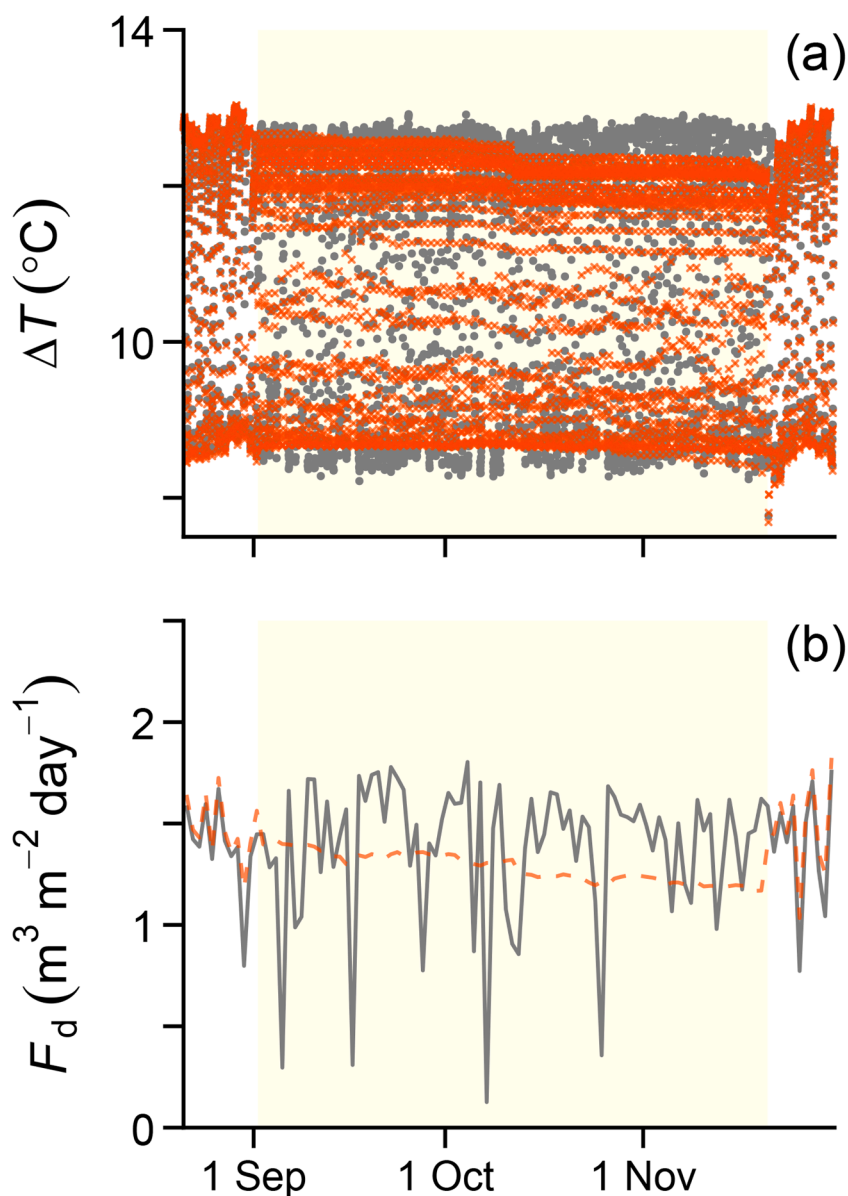


Fig. 4. Output time series comparison between the full and minimum input in the fluxfixer package. Only the period from 21 August to 30 November 2013 was drawn for demonstration purposes. The shaded yellow zones represent periods of long-term missing data due to power supply failures. The full set of input variables includes the time stamps, probe temperature difference (ΔT), precipitation, solar radiation, vapor pressure deficit, air temperature, wind speed, volumetric soil water content, and the time of day. On the other hand, the minimum input includes only the time stamps and ΔT . (a) Gap-filled ΔT half-hourly time series. Output values from the full and minimum input are depicted as gray circles and orange crosses, respectively. (b) Daily sap flux density (F_d) time series calculated using the SP method. The solid gray and orange dashed lines indicate the outputs for the full and minimum inputs, respectively.

only to sap flow data but also to other noisy time series data. For example, raw eddy-covariance flux data also contain high levels of noise and feedback from other meteorological factors; removing outliers and filling gaps in these data could be possible using fluxfixer.

Site managers can use fluxfixer to remove any irregularities in the sap flow observations as soon as they are noticed. When machine learning is used, there is a risk that the accuracy of the estimated values will be reduced if the time series is short, and hence fluxfixer is particularly beneficial for site managers who conduct long-term observations. fluxfixer was released in 2026, and we are currently promoting it to the plant ecophysiology and forest hydrology communities that perform TDM sap flow measurements. fluxfixer has not been used commercially to date, but it has the potential to be incorporated into commercial software provided by companies that sell sap flow sensors and other meteorological instruments.

5. Conclusions

In this paper, we presented fluxfixer, which provides a sophisticated protocol for post-processing TDM sap flow raw time series based on classic statistical and machine-learning methods. This protocol's novelty is that the information from sap flow data and other physical environment factors can be directly used for data correction. We demonstrated the software's utility by processing a long-term, noisy, and unstable ΔT time series observed in a Bornean tropical rainforest. We believe that fluxfixer can significantly impact plant ecophysiology and forest hydrology research, promoting future synthetic analysis. fluxfixer still has room for improvements. This software should be further validated by raw data measured in various types of vegetation. Deciduous forests in particular have transpiration with strong seasonality, and the outlier detection and gap-filling suggested in this paper could be further improved through evaluation on the data of such forests.

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Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the authors used Grammarly Editor to improve readability and linguistic expression. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

CRedit authorship contribution statement

Yoshiaki Hata: Writing – review & editing, Writing – original draft, Visualization, Software, Methodology, Conceptualization. **Tomomi Kumagai:** Writing – review & editing, Supervision, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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