Peters, R. L., Pappas, C., Hurley, A., Poyatos, R., Flo, V., Zweifel, R., Goossens, W., Steppe, K. (2021): Assimilate, process and analyse thermal dissipation sap flow data using the TREXrpackage. - Methods in Ecology and Evolution, 12, 2, 342-350.

https://doi.org/10.1111/2041-210X.13524

Assimilate, process, and analyse thermal dissipation sap flow data using the TREX R package

Richard L. Peters[a,b*], Christoforos Pappas[c,d,e], Alexander G. Hurley[f, g], Rafael Poyatos[h,i], Victor Flo[g], Roman Zweifel[b], Willem Goossens[a], Kathy Steppe[a]

[a]Laboratory of Plant Ecology, Department of Plants and Crops, Faculty of Bioscience Engineering, Ghent University, Coupure links 653, B-9000 Ghent, Belgium

[b]Forest Dynamics, Swiss Federal Research Institute for Forest, Snow and Landscape Research (WSL), Zürcherstrasse 111, CH-8903 Birmensdorf, Switzerland

[c]Département de géographie, Université de Montréal, Montréal, H2V 0B3, Montreal, QC, Canada

[d]Centre d'étude de la forêt, Université du Québec à Montréal, C.P. 8888, Succursale Centre-ville, Montréal, QC, H3C 3P8, Canada

[e]Département Science et Technologie, Téluq, Université du Québec, 5800 rue Saint-Denis, Bureau 1105, Montréal, QC, H2S 3L5, Canada

[g]GFZ German Research Centre for Geosciences, Section 4.3 Climate Dynamics and Landscape Evolution, Potsdam, Germany

[f]School of Geography, Earth and Environmental Sciences, University of Birmingham, Birmingham B15 2TT, United Kingdom

[h]CREAF, E08193 Bellaterra (Cerdanyola del Vallès), Catalonia, Spain

[i]Universitat Autònoma de Barcelona, E08193 Bellaterra (Cerdanyola del Vallès), Catalonia, Spain

*Corresponding Author:

Tel: +32 9 264 61 12, Fax: +32 9 224 44 10, e-mail: Richard.Peters@UGent.be.

Abstract

1. A key ecophysiological measurement is the flow of water (or sap) along the tree's water-transport system, which is an essential process for maintaining the hydraulic connection within the soil-plant-atmosphere continuum. The thermal dissipation method (TDM) is widespread in the scientific community for measuring sap flow and has provided novel insights into water use and its environmental sensitivity, from the tree- to the forest-stand level. Yet, methodological approaches to determine sap flux density (SFD) from raw TDM measurements remains case-specific, introducing uncertainties and hampering data syntheses and meta-analyses.

2. Here, we introduce the R package TREX (TRee sap flow EXtractor), incorporating a wide range of sap flow data-processing procedures to quantify SFD from raw TDM measurements. TREX provides functions for: i) importing and assimilating raw measurements, ii) data quality control and filtering, and iii) calculating standardized SFD outputs and their associated uncertainties according to different data-processing methods.

3. A case study using a Norway spruce tree illustrates TREX's functionalities, featuring interactive data curation and generating outputs in a reproducible and transparent way. The calculations of SFD in TREX can, for instance, use the original TDM calibration coefficients, user-supplied calibration parameters or calibration data from a recently compiled database of 22 studies and 37 species. Moreover, the package includes an automatic procedure for quantifying the sensitivity and uncertainty of the obtained results to user-defined assumptions and parameter values, by means of a state-of-the-art global sensitivity analysis.

4. Time series of plant ecophysiological measurements are becoming increasingly available and enhance our understanding of climate change impacts on tree functioning. TREX allows for establishing a baseline for data processing of TDM measurements and supports comparability between case studies, facilitating robust, transparent, and reproducible large-scale syntheses of sap flow patterns. Moreover, TREX facilitates the simultaneous application of multiple common data-processing approaches from raw data to physiological relevant quantities. This allows for robust quantification of the impact (i.e., sensitivity and uncertainty) of user-specific choices and methodological differences, which is necessary for process understanding and policy making.

Keywords: thermal dissipation method, transpiration, sap flux density, calibration, uncertainty analysis, global sensitivity analysis, whole-tree water use

1 | Introduction

A key ecophysiological measurement is tree water transport, as terrestrial plant transpiration plays a key role in the local, regional and global water cycle (e.g., Reyes-Acosta & Lubczynski 2013; Schlesinger & Jasechko 2014; Fatichi & Pappas 2017). More specifically, sap flow (SF; total flow of water, often expressed in kg H_2O per h) attracts large interest across several scientific disciplines, as it is essential for maintaining the soil-plant-atmosphere continuum (e.g., Zweifel, Item & Häsler 2001; Steppe, Vandegehuchte, Tognetti & Mencuccini 2015). SF can be measured in different plant organs, although it is typically measured in stems. For decades, heat-based SF measurements have been used to quantify whole-tree water use for partitioning ecosystem-level water fluxes into transpiration and evaporation (e.g., Poyatos *et al.* 2016). In addition, species comparisons on stomatal regulation in mature trees have been performed using SF, revealing species-specific environmental responses to drought and heat waves (e.g., Brinkmann, Eugster, Zweifel, Buchmann & Kahmen 2016; Dietrich, Delzon, Hoch & Kahmen 2019).

A large variety of heat-based SF methods exist (as reviewed by Smith & Allen 1996; Peters *et al.* 2018), yet no method suits all needs for tree ecophysiological research. The thermal dissipation method (TDM) is the most widely applied for measuring SF in trees, due to its simplicity and low cost (Flo, Martinez-Vilalta, Steppe, Schuldt & Poyatos 2019). In short, the TDM measures how moving sap within the tree's water conducting xylem (i.e. sapwood) affects the dissipation of heat supplied by a continuous heater (Granier 1985). The TDM is applied by installing two axially aligned probes into the xylem and measuring the temperature difference between a continuously heated probe and the non-heated reference probe (ΔT in °C, or as voltage difference, ΔV in mV) , where ΔT decreases due to the convective cooling with moving sap over the heating probe.

The range of user-specific choices (e.g., parameter values, calculation procedures) applied during data processing between studies represents a key challenge for homogenising and synthesising SF measurements obtained from TDM (Peters *et al.* 2018). A large variety of TDM data-processing steps are applied to convert raw data into physiologically meaningful variables, namely sap flux density (SFD in cm^3 of sap per cm^2 of sapwood area per h), yet often only a single data-processing path is utilized. Typically suggested data-processing steps include: i) determining time periods of zero flow (Rabbel, Diekkrüger, Voigt & Neuwirth 2016), ii) correcting for the partial insertion of the probe into non-conducting heartwood (Clearwater, Meinzer, Andrade, Goldstein & Holbrook 1999), iii) accounting for signal dampening due to wound response (Peters *et al.* 2018), and iv) sensor calibration (Fuchs, Leuschner, Link, Coners & Schuldt 2018). Yet, although data-processing steps can impact the quantification of SFD (Köstner, Granier & Cermák 1998; Peters *et al.* 2018), no consensus exists on a standardized method.

The lack of a standardized method of TDM data processing has stimulated the recent development of software tools for specific TDM data-processing steps (i.e., Oishi, Hawthorne & Oren 2016; Speckman, Ewers & Beverly 2018). Although such tools provide an array of data cleaning procedures with a graphical interface and a fixed chain of data-processing options, they do not facilitate the exploration of multiple approaches and parameter values (i.e., multi-method ensemble for SFD data analyses). Moreover, although there are techniques to identify parameters which critically impact the output of interest (e.g., De Pauw, Steppe & De Baets 2008; Pappas, Fatichi, Leuzinger, Wolf & Burlando 2013), such systematic sensitivity analyses have yet to be considered for TDM data-processing. The consequence is that SFD data from TDM studies may still be difficult to compare or to apply in broader ecological research questions.

Here we present the R package TREX (TRee sap flow Extractor; R Core Team 2017) freely accessible via the Comprehensive R Archive Network (CRAN: http://cran.r-project.org). TREX imports and assimilates raw TDM measurements, provides a complete multi-modular data-processing workflow and facilitates SFD-related outputs and analyses. TREX provides functionalities for interactive data curation, quantification of the sensitivity and uncertainty of the obtained results to user-defined assumptions and parameter values, and produces outputs in a reproducible and transparent way. Notwithstanding, a multitude of the TREX functionalities are also applicable to other heat-based SF measurements.

2 | TREX functionalities

We demonstrate the functionalities of TREX using an example dataset (Figure 1) from a mature Norway spruce (*Picea abies* (L.) Karst.; see *tdm.data*()). TREX functionalities are structured in three modules (Figure 2), where each module contains multiple functions which can be used separately or in a processing chain (short descriptions of the functions are provided in Table S1). The first module "Import & assimilation" guides users to import data, adjust time-step-related issues, perform outlier detection and gap filling. The second module "Data processing" provides a chain of functions which apply different TDM data-processing procedures. The final module "Output & analyses" generates standardized data output and quantifies the output sensitivity and uncertainty associated to variations in selected parameters. Some functions from the "Import & assimilation" and "Output & analyses" modules can also be used with other SF methods (Figure 2).

TREX functions for data import and assimilation

TREX utilizes TDM time series of ΔT (or ΔV) provided for each individual sensor in text file format, with ΔT (or ΔV) data recorded for a specific timestamp, providing information on time zone and daylight saving time (see *example.data*()). It is crucial to know the time zone in which the data were logged and whether day-time-saving was applied. The input can be presented in a *Timestamp* format: including a timestamp of the measurements column, and value of ΔT (or ΔV) of a specific sensor (Table 1; but also see *DOY* format in *?TREX::example.data)*. Multiple reference probes used to correct for natural temperature gradients in the sapwood (Lindén, Fonti & Esper 2016) can also be added as additional columns (labelled as *ref1*, *ref2*, …, *refn*). The user can verify whether the imported dataset fits the requirements for TREX data format by calling the function *is.trex*(). After specifying the timestamp format and time zone, the users can select whether the time series should be standardized to solar time (i.e., mid-day corresponding to solar noon which enhances comparability across sites) by providing the longitude (in decimal degrees) of the location of the sensor. Although TREX functionalities are applied per individual sensor, a looping procedure could allow for analysing multiple individual trees or sensors.

The *dt.steps*() function manipulates the temporal extent and resolution (indicated with *time.int* in minutes) of an *is.trex* object (i.e., to facilitate comparison with other time series). Outliers in ΔT (or ΔV) time series need to be identified and removed before proceeding with data processing (Figure 3). This task is addressed in the TREX package with an accompanying Shiny application that is launched with the *outlier*() function and i) visualizes raw and outlier-free time series interactively (Sievert 2018), ii) highlights automatically detected outliers (see ?*TREX*::*outlier*() for method specifications), iii) allows the user to revise the automatically detected outliers and manually include data points interactively, and iv) exports the original data and the outlier-free time series in a *is.trex*() object that can be further processed. The cleaned or raw time series can additionally be fed to the *gap.fill*() function to interpolate sporadic gaps of a user-defined length (using *max.gaps* defined in minutes).

TREX data-processing functions

SFD is estimated by first determining the relative thermal difference (known as the heat index and denoted as K, unitless) between ΔT and zero-flow conditions (denoted as ΔT_{max} or ΔV_{max} in equation 1; Granier 1985). Multiple methods exist to determine ΔT_{max} (equation 1; Rabbel, Diekkrüger, Voigt & Neuwirth 2016). Four classes of methods (as reviewed by Peters *et al.* 2018) are incorporated in the function *tdm_dt.max*(), including: i) the pre-dawn ΔT_{max} (*pd*), where zero-flow is assumed to occur each night, ii) daily moving window (*mw*; e.g., 7 days, defined with *max.days*), in which the centred maximum pre-dawn ΔT_{max} over a moving window is assumed to represent zero-flow conditions, iii) the double regression method (*dr*; Lu, Urban & Zhao 2004), determining the mean pre-dawn ΔT_{max} over the *max.days* period and removes all points below this moving-window mean and calculates a second running mean moving window, and iv) the environmental dependent method (*ed*) assuming that one can find zero-flow conditions based on environmental conditions (Oishi, Hawthorne & Oren 2016; see *?TREX::tdm_dt.max* for details). As the selected parameters are likely site-, and even tree-specific, users should carefully inspect the selected nights of zero-flow conditions resulting from the selected criteria (e.g., Figure S1). Yet, when determining ΔT_{max}, users have to keep in mind that it is a subjective process where the four presented methods may not be suitable for all regions or tree species. For example, in some regions where zero-flow conditions do not occur over many weeks, an alternative approach needs to be sought. Moreover, zero-flow conditions might not be homogeneous across the radial profile of the sapwood, which may require a different ΔT_{max} method for the inner- *versus* outer-sapwood.

Equation 1.

$$K = \frac{\Delta T_{max} - \Delta T}{\Delta T}$$

The correction for the proportion of the probe that is inserted into the non-conducting heartwood is another important data-processing step (see Peters *et al.* 2018). This correction is incorporated in the *tdm_hw.cor*() function using the sapwood thickness (*sapwood.thickness* in mm). Together with the length of the probe (*probe.length* in mm), the proportion of the probe inserted into the sapwood (γ in mm mm^{-1}) *vs.* the proportion of the probe in the inactive heartwood is used to calculate ΔT_{sw} (Equation 2) which replaces ΔT (Equation 1; Clearwater, Meinzer, Andrade, Goldstein & Holbrook 1999).

Equation 2 $$\Delta T_{\mathrm{sw}} = \frac{(\Delta T - (1-\gamma) \cdot \Delta T_{\mathrm{max}})}{\gamma}$$

The installation of probes into living tissues results in signal dampening in *K* that is particularly pronounced in multi-annual observation periods (see Wiedemann, Marañón-Jiménez, Rebmann, Herbst & Cuntz 2016). When probes are inserted into the xylem without reinstalling each year, one can correct for the dampening effect with the statistical method proposed by Peters *et al.* (2018) with the *tdm_damp*() function. Yet, it should be noted that no empirical evidence (i.e., gravimetric validation) exists to confirm the correction shape of this function and should thus be implemented with caution. Moreover, such data-driven statistical approach may hamper data analyses related to inter-annual variability. Moreover, more mechanistic approaches are needed to address this issue and improve the accuracy of the approaches to correct for signal dampening. For *K* values obtained from preceding functions, a dampening model can be fitted to calculate corrected *K* values (using *nls*(); equation 3 and see *?TREX::tdm_damp* for details). After careful visual inspection of the fitted model, the fitted parameters (*a*, *b*, *c*, and *d*) can be used to correct *K* and scaled to the maximum values within the first year since installation (Figure 4).

Equation 3 $$K_{\mathrm{res}} = \frac{(a + b \cdot t)}{(1 + c \cdot t + d \cdot t^2)}$$

SFD is defined by the relationship between *K* and SFD using a power-type function (equation 4). Recent calibration studies and meta-analyses have urged the application of case- or species-specific calibration experiments (e.g., Steppe, De Pauw, Doody & Teskey 2010; Fuchs, Leuschner, Link, Coners & Schuldt 2018; Flo, Martinez-vilalta, Steppe, Schuldt & Poyatos 2019). Thus, within the *tdm_cal.sfd*() one can either supply raw calibration experiment data or provide *a* and *b* parameters from the obtained calibration experiments (equation 4). Alternatively, the package also contains a database of raw calibration measurements, from 22 studies covering 37 species covering the main wood anatomy types, (Flo, Martinez-vilalta, Steppe, Schuldt & Poyatos 2019; Figure 5; see *cal.data*).

Equation 4. $$\mathrm{SFD} = a \cdot K^b$$

3 | TREX uncertainty and sensitivity analyses and output generation

Uncertainty and sensitivity analyses

Each parameter choice in TDM data-processing affects the SFD output. The uncertainty, i.e., variability in relevant SFD output caused by input parameters used in the data-processing cascade, could impact the level of confidence in tree water-use estimates which is relevant for both, mechanistic understanding of ecophysiological processes and environmental decision making (Maier, Ascough, Wattenbach, Renschler & Labiosa 2008). Besides providing a framework to quantify uncertainty, assessing the contribution of specific input parameters to the overall output uncertainty could support the identification of key parameters, that could be better constrained with additional data collection, and thus reducing the final output uncertainty (e.g., Pappas, Fatichi, Leuzinger, Wolf & Burlando 2013).

The *tdm_uncertain*() function performs uncertainty and global sensitivity analysis of TDM time series (using the Sobol's total sensitivity indices as implemented in the "sensitivity" R package; Iooss, Janon & Pujol 2019; see Note S1 for details). For conducting sensitivity and uncertainty analyses of TDM data with TREX, the user needs to: i) select the output variable of interest, ii) identify the relevant input parameters (some of them are method-specific), and iii) determine their range and statistical distributions (Table 2). For a given time series three output variables are considered, calculated as the mean over the entire time period where data are available, namely: i) mean daily sum of water use ("Sum", expressed as SFD or *K*), ii) the variability in maximum SFD or *K* values ("CV", coefficient of variation in % as this alters climate response correlations), and iii) the duration of daily sap flow based on SFD or *K* below a user-defined threshold ("Duration", expressed in hours per day dependent on a threshold, see *min.sfd* and *min.k*). The relevant input parameters are presented for each of the ΔT_{max} methods in Table 2, (providing default values and sampling distributions; excluding *tdm_damp*() as its application demands detailed visual inspecting). Yet, users should note that parameter ranges and distributions represent an important critical component of any sensitivity analysis and should be carefully assessed (Wallach & Genard 1998).

The *tdm_uncertain*() function provides both graphical (Figure 6) and tabular output (Table S2) depending on the ΔT_{max} calculation method (Figure S2-S3). The sensitivity output for each ΔT_{max} calculation method can be compared to identify key parameters which need to be constrained. In the Norway spruce example dataset, the total sensitivity indices for the Sum, CV and Duration based on *K* values illustrate that both the Sum and CV of *K* are highly sensitive to the sapwood correction, suggesting the need for carefully establishing sapwood depth at the location of probe installation (Figure 6). For all outputs based on SFD the *b* parameter of the power-type calibration curve appears to strongly impact both absolute water flow as well as their variability, illustrating the need for robust calibration curves to constrain the output variables. High sensitivity of CV to some of the input parameters suggests potential alterations of SF environmental responses caused by methodological variability (Peters *et al*. 2018).

Relevant output generation

The package provides the functionality to temporarily aggregate the required SFD data into any user-defined interval (*agg.data*(); e.g., daily sap flow values in cm^3 cm^{-2} d^{-1}). Moreover, the package provides the *out.data*() function to generate either SFD (expressed as F_d in mmol m^{-2} s^{-1}) or crown conductance estimates (G_C in cm^3 cm^{-2} h^{-1} kPa^{-1}) outputs in an exportable format. Here, G_C is defined as the ratio of SFD to VPD and is analogue to stomatal conductance under conditions of negligible stem capacitance, but expressed per unit of sapwood area (Meinzer *et al.* 2013). The function *out.data*() offers the opportunity to decide about the conditions that fulfil these negligible capacitance assumptions (see Note S2 for details). A non-linear model of the form $G_C = \alpha + \beta\ VPD^{-0.5}$ can then be automatically fitted with the *out.data*() function to the selected peak-of-day mean values of G_C on VPD to quantitatively describe the observed patterns (Figure S4; as described in Pappas *et al.* 2018). This can be used to get preliminary insights into tree water use strategies, yet caution is needed for the interpretations of these values (i.e., capacitance assumptions need to be verified and G_C response models to VPD have statistical limitations due to estimation of G_C using VPD).

4 | Conclusion

The TREX package contains advanced functionalities to assimilate, process and analyse raw sap flow measurements obtained with the TDM. The package provides means for transparent and reproducible TDM data processing and for enhancing comparability of SFD estimates between studies. Moreover, to our knowledge, this is the first study to provide a state-of-the-art systematic quantification of sap flow uncertainty and sensitivity due to data-processing parameter inputs and assumptions. We believe that TREX provides a structured and transparent pathway for sap flow data processing, which will emphasize the utility of heat-based sap flow measurements for future research. The package structure eases the implementation of future processing methods when made available from the scientific community, facilitating thus multi-method comparisons and robust sensitivity and uncertainty analyses.

Acknowledgements

We thank Patrick Fonti for providing constructive comments on an earlier version of the manuscript and supplying the example dataset collected at the Lötschental transect. We thank Dirk J. W. De Pauw and Ana Stritih for their discussions on uncertainty analyses. We also thank all researchers and their funding agencies, whose work was essential for obtaining all the calibration experiment data. RLP acknowledges the support of the Swiss National Science Foundation (SNSF), Grant P2BSP3_184475. CP acknowledges the support of the SNSF (Grants P2EZP2_162293 and P300P2_174477), the Canada Research Chair in Atmospheric Biogeosciences in High Latitudes and the Global Water Futures project Northern Water Futures. RP acknowledges the support of the Spanish grant RTI2018-095297-J-I00 and of a Humboldt Research Fellowship for Experienced Researchers. Data collection was performed in the framework of the SNSF projects INTEGRAL (121859) and LOTFOR (150205). All authors declare that there is no conflict of interest,

Data availability statement

The TREX package is available as a package in R. The program R is freely available from the Comprehensive R Archive Network (CRAN; http://cran.r-project.org/). The package and presented example data is also available for download and installation via a GitHub (https://github.com/the-Hull/TREX) and Zenodo (http://doi.org/10.5281/zenodo.4121258) repository.

Authors' Contributions

RLP, CP and AGH initiated the concept of the R package TREX and developed the main functions. RP and VF aided in further developing the functionalities and AH mainly compiled the R package. RLP and KS raised the funding. RLP and CP wrote the manuscript and all authors contributed to the manuscript drafts.

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Figure legends

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Figure 5. Calibration curves obtained from literature, including all wood types (using the *tdm_cal.sfd*() function; mean [μ] and confidence interval [CI] over studies). The grey background shows the *K* range of the specific zero flow method, which was provided as input for the function and illustrates whether the uncertainty of the calibration curve (presented with CI) will impact the *K* time series.

Figure 6. Visual output from the *tdm_uncertain*() function when considering the double-regression ΔT_{max} method for the Norway spruce example dataset (see Figure 1). Total Sobol' sensitivity indices of the investigated parameters with their mean (coloured dots) and 95% confidence intervals (vertical lines) are provided for *K* and SFD, respectively (see Note S1 for details). The sensitivity analysis was conducted on the example dataset considering the time window May to November of 2013. Less parameters are presented for *K* as the calibration parameters (*a* and *b* in equation 2) do not affect *K*. The smaller panels on the right present the uncertainty over the selected output variables. 'Sum' indicates the daily sum of water use (expressed in cm^3 cm^{-2} d^{-1} for SFD or unitless for *K*), 'CV' the variability of maximum SFD or *K* values (coefficient of variance in %), and 'Duration' the duration of daily transpiration based on SFD or *K* (expressed in h per day dependent on a threshold).

Tables

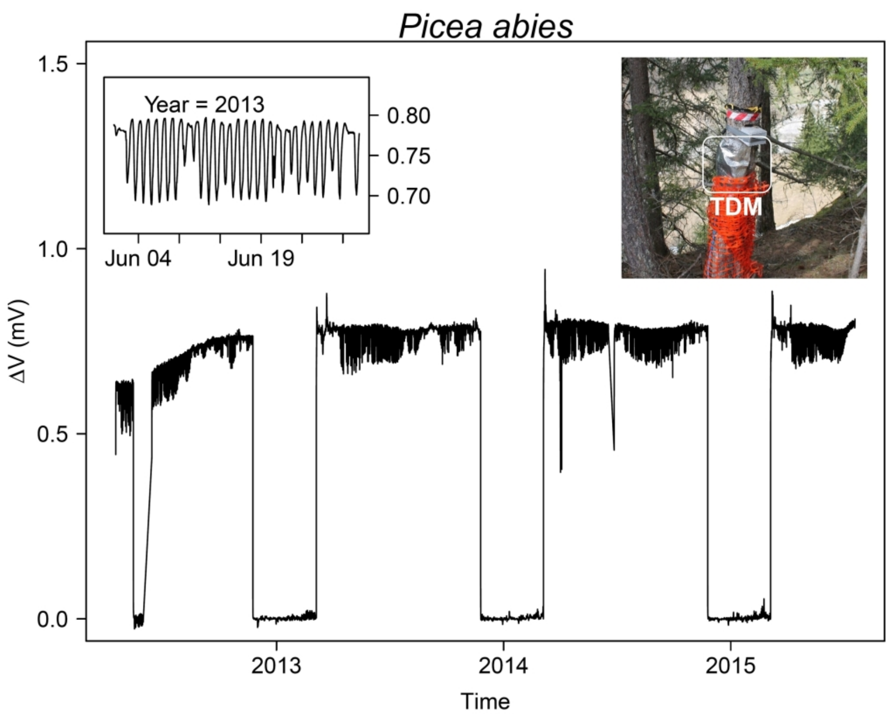
Table 1. Example of TREX data format of a thermal dissipation time series *example.data*(*type*= "timestamp"). Data of an individual tree has to be provided, including timestamp and value (in ΔT or ΔV; here ΔV).

timestamp	value
17-4-2012 15:00	0.444
17-4-2012 15:15	0.541
17-4-2012 15:30	0.560
17-4-2012 15:45	0.568
17-4-2012 16:00	0.572
17-4-2012 16:15	0.545
…	…

Table 2. Selection of data-processing parameters relevant for the uncertainty and sensitivity analyses. Each ΔT_{max} method is considered with its unique set of parameters (indicated with square brackets). Default values incorporated into TREX, operating on the example dataset, are provided as a baseline and are based on expert judgement and existing literature. Incorporated data-processing functions include: *tdm_dt.max*() calculating zero-flow conditions, *tdm_hw.cor*() implementing the heartwood correction, and *tdm_cal.sfd*() quantifying the sap flux density. The ΔT_{max} methods include: pre-dawn (pd), moving window (mw), double regression (dr) and environmental dependent (ed).

Data-processing [ΔT_{max} method]	Parameter	Sampling distribution	Default values
tdm_dt.max[pd/mw/dr/ed]	zero.start	Integer sampling range	2 hours
	zero.end	Integer sampling range	2 hours
tdm_dt.max[mw/dr]	max.days	Integer fixed sampling range	5-15 days
tdm_dt.max[ed]	ed.window	Integer fixed sampling range	2-4 hours
	criteria[sr]	Dependent sampling range	30%
	criteria[vpd]	Fixed sampling range	0.05-0.5 kPa
	criteria[cv]	Fixed sampling range	0.5-1 %
tdm_hw.cor [pd/mw/dr/ed]	sapwood.thickness [sw.cor]	Normal distribution	σ =16 mm
tdm_cal.sfd [pd/mw/dr/ed]	a	Normal distribution (Log)*	μ=4.085; σ= 0.628
	b	Normal distribution*	μ=1.275; σ= 0.262

*See *cal.sfd* with Use all; Coniferous in example



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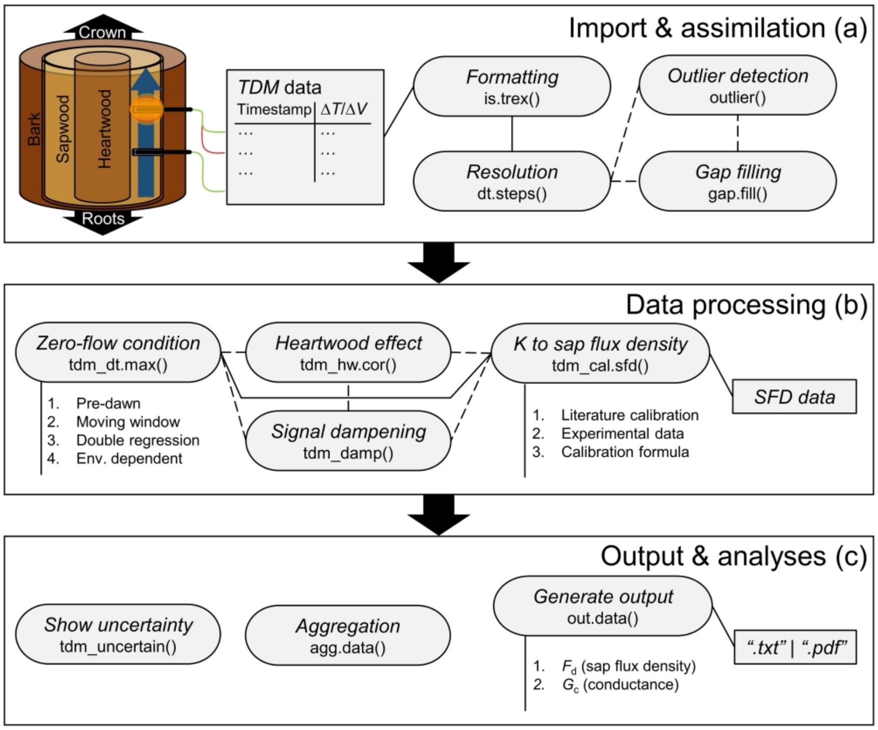
254x190mm (300 x 300 DPI)



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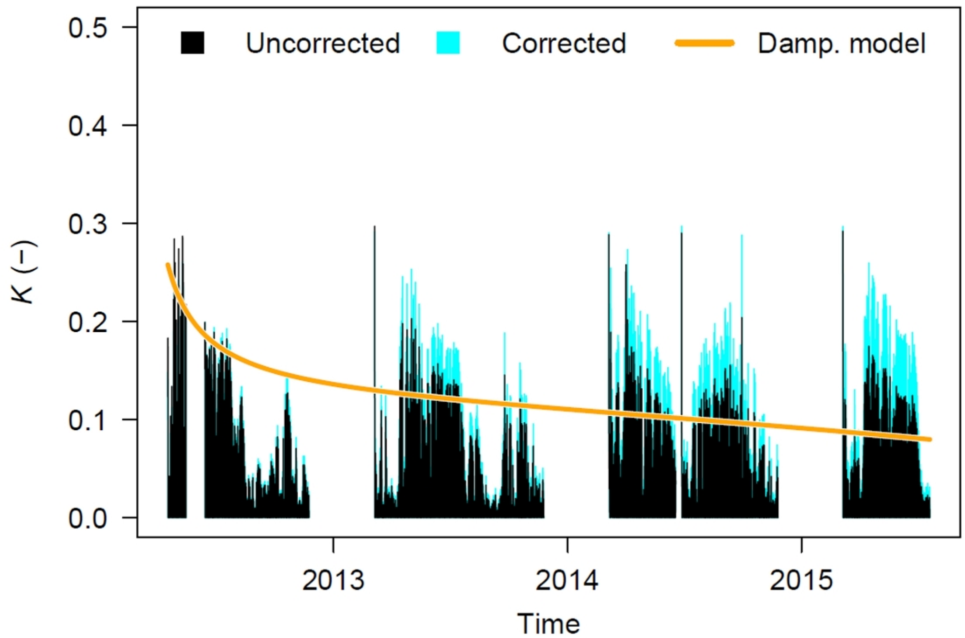

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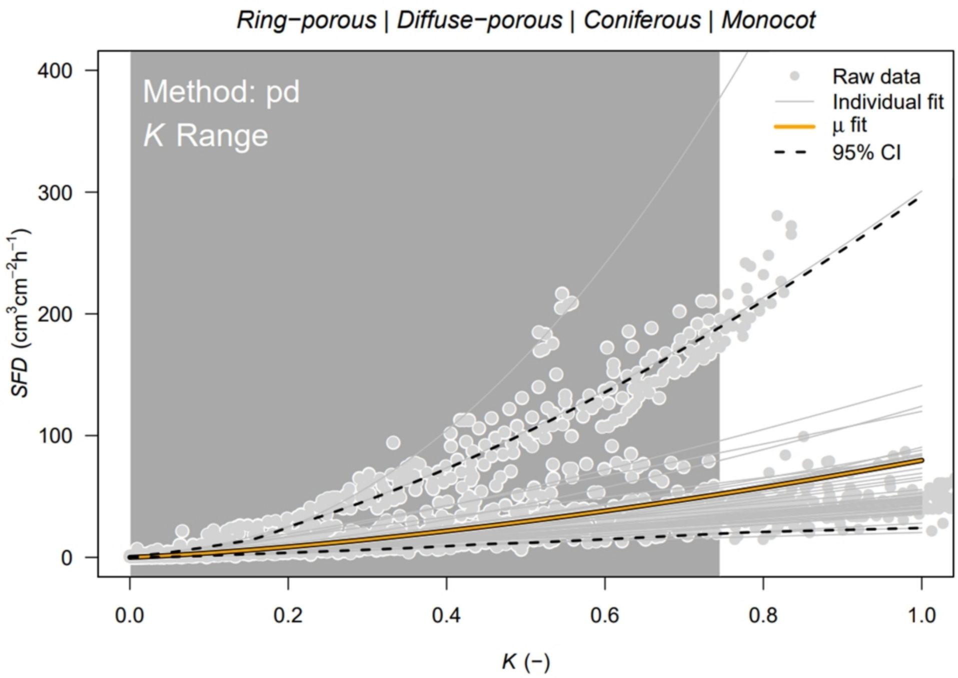

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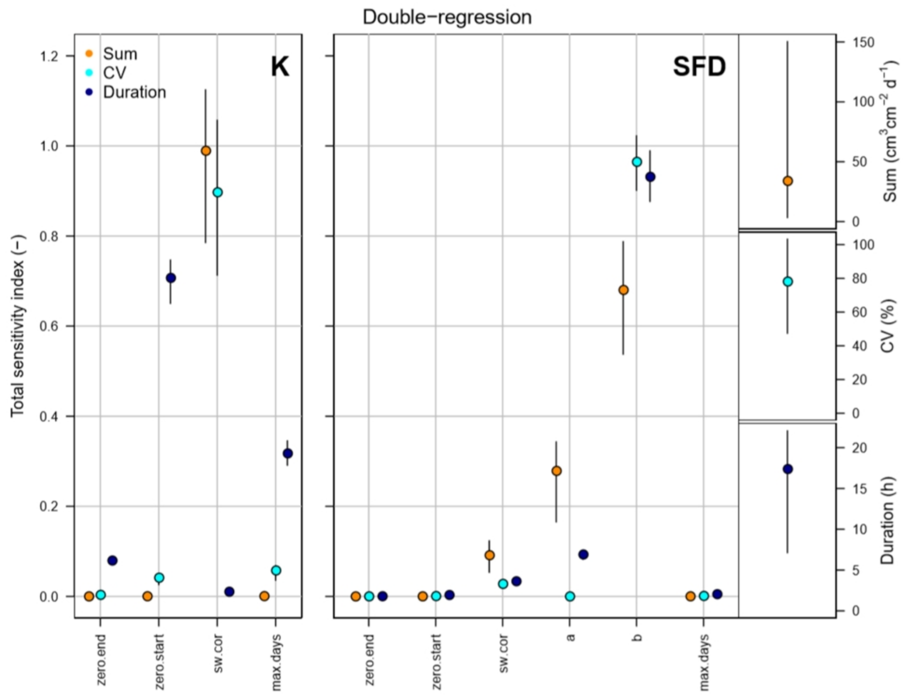

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