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APPLICATION

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

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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 remain 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 (a) importing and assimilating raw measurements, (b) data quality control and filtering and (c) 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 to convert 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 assumptions, which is necessary for process understanding and policy making.

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

1 | INTRODUCTION

A key ecophysiological measurement is tree water transport, as terrestrial plant transpiration plays a crucial role in the local, regional and global water cycle (e.g. Fatichi & Pappas, 2017; Reyes-Acosta & Lubczynski, 2013; Schlesinger & Jasechko, 2014). More specifically, sap flow (SF; total flow of water, often expressed in kg H_2O per hr) attracts large interest across several scientific disciplines, as it is essential for maintaining the soil–plant–atmosphere continuum (e.g. Steppe et al., 2015; Zweifel et al., 2001). 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 et al., 2016; Dietrich et al., 2019).

A large variety of heat-based SF methods exist [as reviewed by Peters et al. (2018) and Smith and Allen (1996)], 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 et al., 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 homogenizing and synthesizing 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 hr), yet often only a single data-processing path is utilized. Typically suggested data-processing steps include (a) determining time periods of zero sap flow (Rabbel et al., 2016), (b) correcting for the partial insertion of the probe into non-conducting heartwood (Clearwater et al., 1999), (c) accounting for signal dampening due to wound response (Peters et al., 2018) and (d) sensor calibration (Fuchs et al., 2017). Yet, although data-processing steps can impact the quantification of SFD (Köstner et al., 1998; Peters et al., 2018), no consensus exists on a standardized sap flow processing 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 et al., 2016; Speckman et al., 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 et al., 2008; Pappas et al., 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: https://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

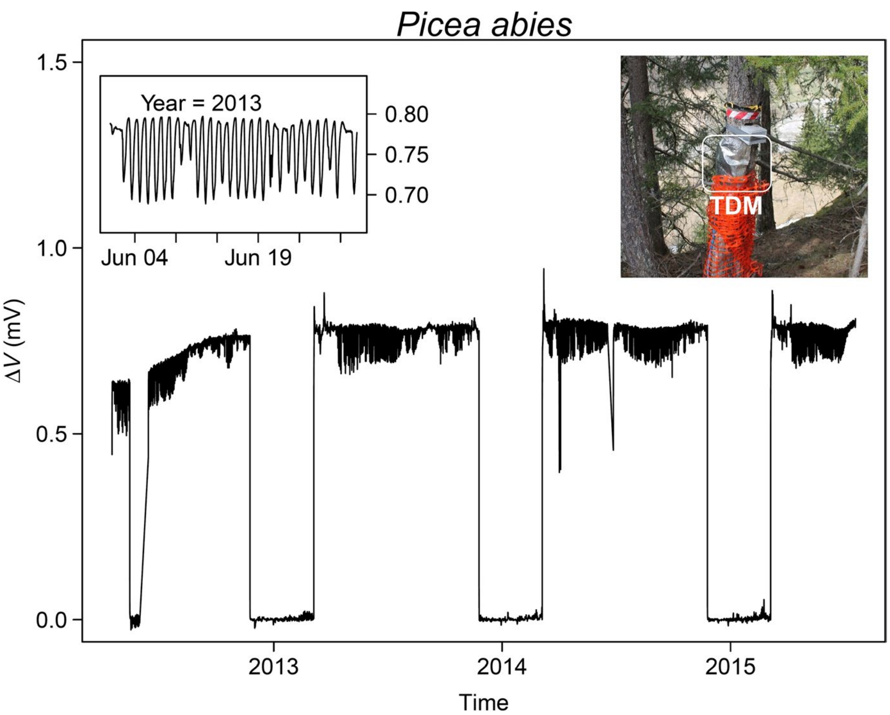

FIGURE 1 Example of a thermal dissipation method (TDM) time series from a mature Norway spruce (*Picea abies* Karst.) growing in an alpine valley at 1,300 m a.s.l. (Lötschental, Switzerland; Peters et al., 2019)

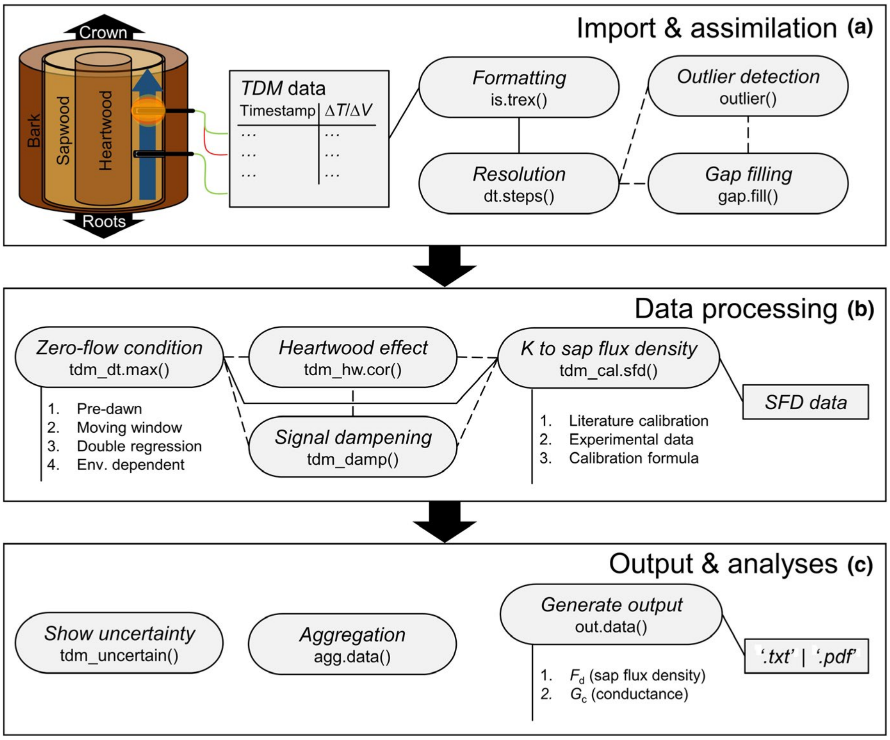

FIGURE 2 Schematic overview of the modules (a–c), functions and workflow of the TREX (TRee sap flow EXtractor) package. Functions which are specifically designed to work with thermal dissipation method data are indicated with 'tdm_...' while other functions can be applied on any type of sap flow data

& 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 with variations in selected parameters. Some functions from the 'Import & assimilation' and 'Output & analyses' modules can also be used with other SF methods (Figure 2).

2.1 | 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 *?example.data*()). Multiple reference probes used to correct for natural temperature gradients in the sapwood (Lindén et al., 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 sensors.

TABLE 1 Example of TREX (TRee sap flow EXtractor) data format of a thermal dissipation time series *example.data*(*type*= 'timestamp'). Data of an individual tree have 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
...	...

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

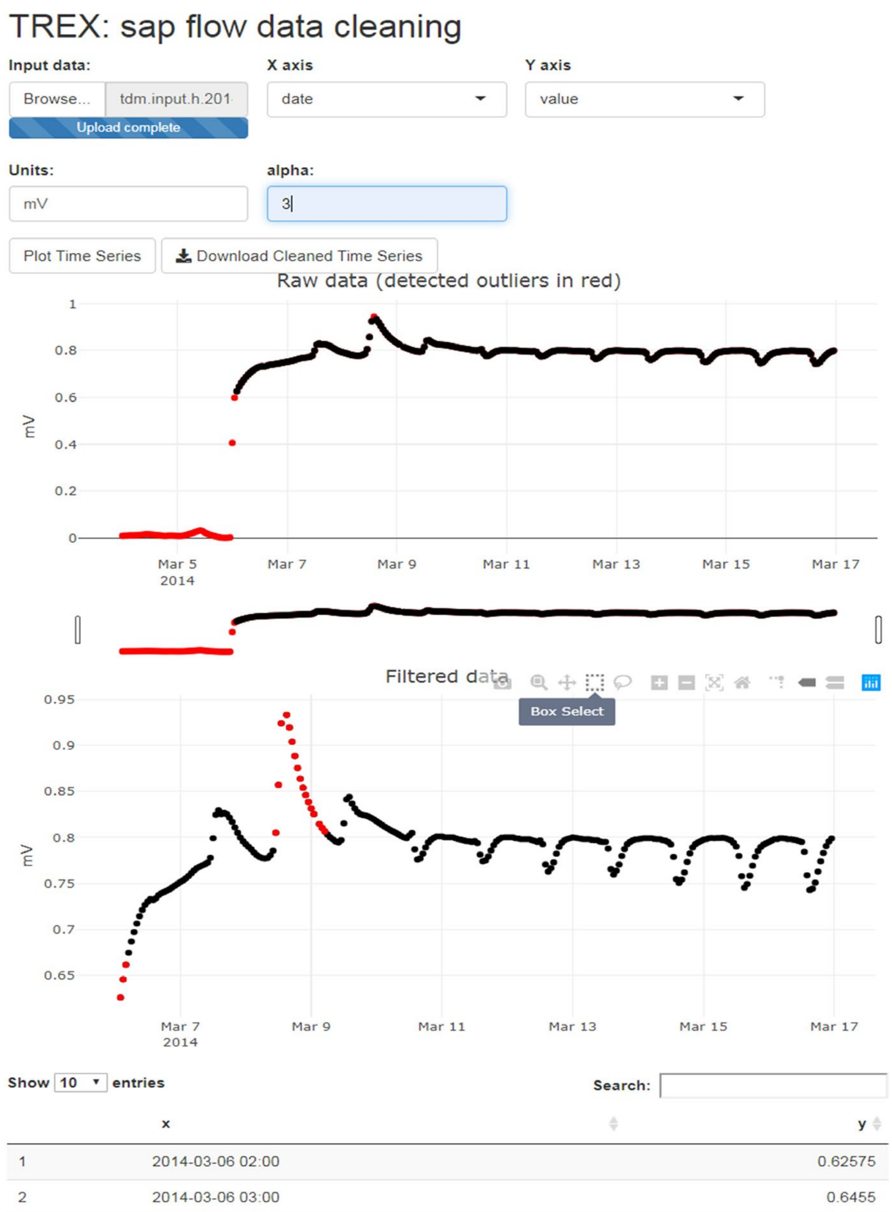

FIGURE 3 An illustration of the *outlier*() function, launching a Shiny application for interactive time series visualization and inspection. Users can adjust the *alpha* parameter for the automatic detection of outliers. Red points in the upper panel highlight the automatically detected outliers, whereas red points in the lower panel are manually selected points

the TREX package with an accompanying Shiny application that is launched with the *outlier*() function and (a) visualizes raw and outlier-free time series interactively (Sievert, 2018), (b) highlights automatically detected outliers (see ?*outlier*() for method specifications), (c) allows the user to revise the automatically detected outliers and manually include data points interactively and (d) 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).

2.2 | TREX data-processing functions

Sap flux density 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 et al., 2016). Four classes of methods (as reviewed by Peters et al., 2018) are incorporated in the function *tdm_dt.max*(), including (a) the pre-dawn ΔT_{max} (*pd*), where zero-flow is assumed to occur each night, (b) 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, (c) the double regression method (*dr*; Lu et al., 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 (d) the environmental-dependent method (*ed*) assuming that one can find zero-flow conditions based on environmental conditions (Oishi et al., 2016; see ?*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.

$$K = \frac{\Delta T_{max} - \Delta T}{\Delta T}. \qquad (1)$$

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) versus the proportion of the probe in the inactive heartwood is used to calculate ΔT_{sw} (Equation 2) which replaces ΔT (in Equation 1; Clearwater et al., 1999).

$$\Delta T_{sw} = \frac{\left(\Delta T - (1-\gamma)\cdot \Delta T_{max}\right)}{\gamma}. \qquad (2)$$

The installation of probes into living tissues results in signal dampening in K that is particularly pronounced in multi-annual observation periods (see Wiedemann et al., 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 ?*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).

$$K_{res} = \frac{(a + b\cdot t)}{\left(1 + c\cdot t + d\cdot t^2\right)}. \qquad (3)$$

Sap flux density 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. Flo et al., 2019; Fuchs et al., 2017; Steppe et al., 2010). Thus, within the *tdm_cal.sfd*(), one can either supply raw calibration experiment data or provide a and b

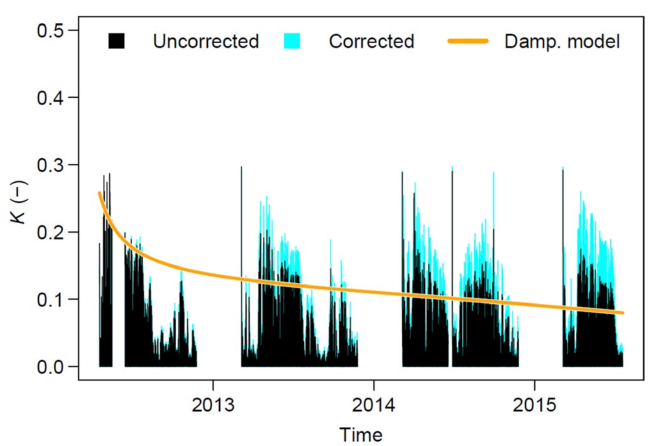

FIGURE 4 Example of the dampening model function to correct K (using the *tdm_damp*() function) for the Norway spruce example dataset (see Figure 1). As a smooth curve is fitted and it shows good agreement with the maximum values over the years presented, we consider this an appropriate correction

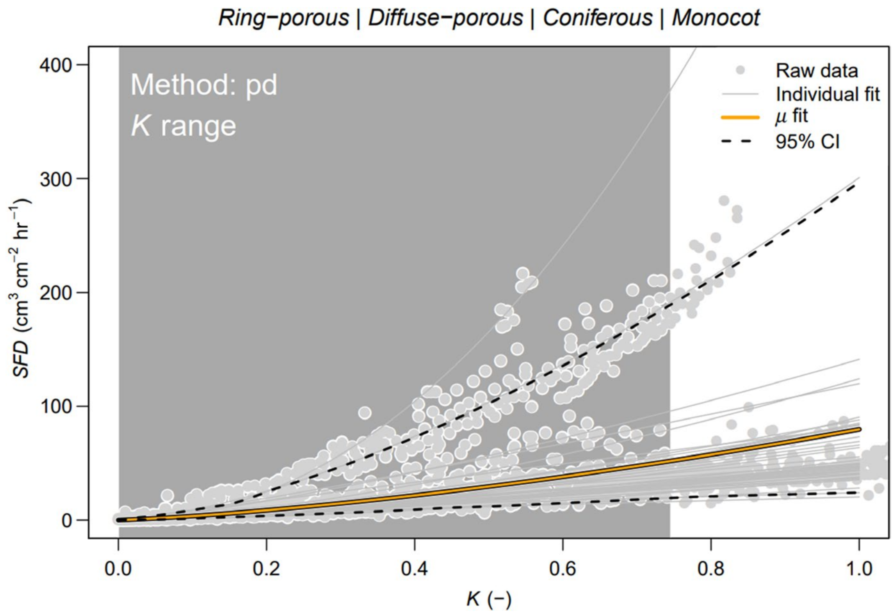

FIGURE 5 Calibration curves obtained from literature, including all wood types (using the *tdm_cal.sfd*() function; mean [μ] and confidence interval [CI] over studies). The grey background shows the K range of the specific zero flow method, which was provided as input for the function and illustrates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

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 et al., 2019; Figure 5; see *?cal.data*).

$$\mathrm{SFD} = a \cdot K^{b}. \quad (4)$$

3 | TREX UNCERTAINTY AND SENSITIVITY ANALYSES AND OUTPUT GENERATION

3.1 | Uncertainty and sensitivity analyses

Each parameter choice in TDM data-processing affects the SFD output. The uncertainty, that is, 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 et al., 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 reduce the final output uncertainty (e.g. Pappas et al., 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 et al., 2019; see Note S1 for details). For conducting sensitivity and uncertainty analyses of TDM data with TREX, the user needs to (a) select the output variable of interest, (b) identify the relevant input parameters (some of them are method-specific) and (c) 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 (a) mean daily sum of water use ('Sum', expressed as SFD or K), (b) the variability in maximum SFD or K values ('CV', coefficient of variation in % as this alters climate response correlations) and (c) 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 (Figures S2 and S3). The output of the sensitivity analysis 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 and 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).

3.2 | Relevant output generation

The package provides the functionality to temporarily aggregate the required SFD data into any user-defined interval (see *?agg.data*(); e.g. daily sap flow values in $cm^3\ cm^{-2}\ d^{-1}$). Moreover, the

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 hr
	zero.end	Integer sampling range	2 hr
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 hr
	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	$\sigma = 16$ mm
tdm_cal.sfd [pd/mw/dr/ed]	a	Normal distribution (Log)[a]	$\mu = 4.085$; $\sigma = 0.628$
	b	Normal distribution[a]	$\mu = 1.275$; $\sigma = 0.262$

[a]See *tdm_cal.sfd* using all wood types.

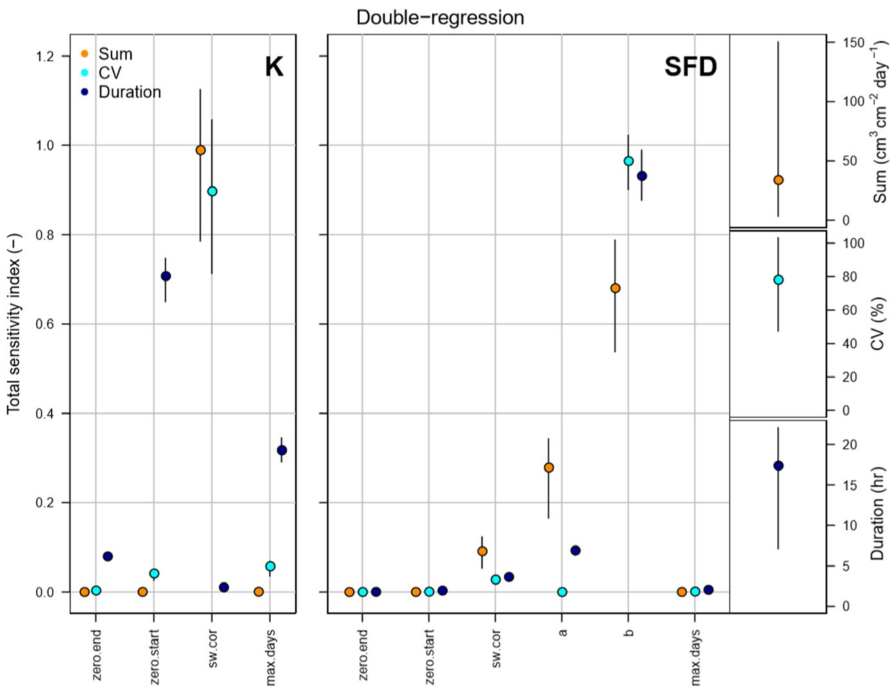

FIGURE 6 Visual output from the *tdm_uncertain*() function when considering the double-regression ΔT_{max}method for the Norway spruce example dataset (see Figure 1). Total Sobol sensitivity indices of the investigated parameters with their mean (coloured dots) and 95% confidence intervals (vertical lines) are provided for *K* and sap flux density (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 4) 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)

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} hr^{-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 nonlinear 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, thus facilitating multi-method comparisons and robust sensitivity and uncertainty analyses.

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AUTHORS' CONTRIBUTIONS

R.L.P., C.P. and A.G.H. initiated the concept of the R package TREX and developed the main functions; R.P. and V.F. aided in further developing the functionalities and A.G.H. mainly compiled the R package; R.L.P. and K.S. raised the funding; R.L.P. and C.P. wrote the manuscript and all authors contributed to the manuscript drafts.

PEER REVIEW

The peer review history for this article is available at https://publons.com/publon/10.1111/2041-210X.13524.

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 are also available for download and installation via a GitHub (https://github.com/the-Hull/TREX) and Zenodo http://doi.org/10.5281/zenodo.4121258 (Peters et al., 2020) repository.

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section.

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