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SHORT COMMUNICATION

TRACC: an open source software for processing sap flux data from thermal dissipation probes

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Abstract

Key message **TRACC is an open-source software for standardizing the cleaning, conversion, and calibration of sap flux density data from thermal dissipation probes, which addresses issues of nighttime transpiration and water storage.**

Abstract Thermal dissipation probes (TDPs) have become a widely used method of monitoring plant water use in recent years. The use of TDPs requires calibration to a theoretical zero-flow value (ΔT_0); usually based upon the assumption that at least some nighttime measurements represent zero-flow conditions. Fully automating the processing of data from TDPs is made exceedingly difficult due to errors arising from many sources. However, it is desirable to minimize variation arising from different researchers' processing data, and thus, a common platform for processing data, including editing raw data and determination of ΔT_0, is useful and increases the transparency and replicability of TDP-based research. Here, we present the TDP data processing software TRACC (Thermal dissipation Review Assessment Cleaning and Conversion) to serve this purpose. TRACC is an open-source software written in the language R, using graphical presentation of data and on screen prompts with yes/no or simple numerical responses. It allows the user to select several important options, such as calibration coefficients and the exclusion of nights when vapor pressure deficit does not approach zero. Although it is designed for users with no coding experience, the outputs of TRACC could be easily incorporated into more complex models or software.

Keywords Thermal dissipation probes · Sap flux · Ecohydrology · Open source software · Transpiration

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Thermal dissipation probe calibration

Thermal dissipation probes (TDPs; (Granier 1987)) have become a widely used method of monitoring plant water use in recent years (Lu et al. 2004). The underlying basis of these measurements is the measurement of a temperature difference between two cylindrical probes inserted radially into the sapwood of a tree, one above the other. The upper probe is heated with a constant power output and establishes the temperature difference, which declines as water flows past the heated probe. The probe set contains a type T (copper-constantan) differential thermocouple with a junction in each probe that produces a signal on the order of hundreds of millivolts, which is converted into a temperature difference measurement (ΔT_M). This signal is then translated to a sap flux density (J_S) in units of g H_2O m^{-2} sapwood s^{-1} using a calibration in the form:

$$J_S = \alpha K^{\beta}, \quad (1)$$

where α and β are empirically derived coefficients, while K is the normalized difference between the temperature differential ($\Delta T_{M(t)}$) at time of measurement (t) and a theoretical differential at zero J_S ($\Delta T_{0(t)}$) in the form:

$$K_{(t)} = \left(\Delta T_{0(t)} - \Delta T_{M(t)}\right)/\Delta T_{M(t)}. \quad (2)$$

Originally, it was widely held that a single calibration could be used for all woody plants. In recent years, some evidence has emerged that the values of α and β may differ between species (Bush et al. 2010; Steppe et al. 2010; Sun et al. 2012). However, it has generally been found that this relationship between K and J_S (Eq. 1) is adequate to describe observations (Goulden and Field 1994; McCulloh et al. 2007) with most studies concluding a recalibration of α and β or simple linear correction is all that is needed for species that diverge from the original calibration (Granier 1985, 1987). A modeling study (Wullschleger et al. 2011) suggests that thermal properties of sap wood, wounding responses, and radial variation in sap flux density may all play a role in these calibrations and there is some laboratory evidence that stem water content may play a role in field conditions (Vergeynst et al. 2014).

Several approaches to determining an appropriate value for ΔT_0 have been employed in past studies, many of which are summarized in Lu et al. (2004). Most of these approaches are based upon the assumption that at least some nighttime values of ΔT_M represent zero-flow conditions and thus provide estimates of ΔT_0 that may be used to produce a time-series, $\Delta T_{0(t)}$, for all measurement intervals, either by interpolation or regression. If predawn values of ΔT_M are assumed to represent zero J_S on all nights, they can either be used as ΔT_0 for the following 24 h or linearly interpolated between subsequent days.

However, in the past decade, increasing awareness of non-zero nighttime transpiration (Green et al. 1989; Caird et al. 2007; Dawson et al. 2007; Fisher et al. 2007) that can prevent zero flow conditions (Donovan et al. 1999; Sellin 1999; Donovan et al. 2001; Kavanagh et al. 2007) has led to the exclusion of nights when vapor pressure deficit (VPD) does not reach or approach zero [e.g., (Oishi et al. 2008)]. Diurnal fluctuations in water storage of woody tissues [i.e., hydraulic capacitance (Phillips et al. 1997, 2004; Goldstein et al. 1998; Meinzer et al. 2003; Cermak et al. 2007)] may require that such conditions be met for a substantial amount of time to allow the establishment of zero-flow at sensor height, which may be some distance from leaves. This ensures minimal evaporative demand (and thus transpiration) for a period deemed long enough for the water potential gradient within the tree to approach equilibrium.

Nocturnal sap flow has been demonstrated in many studies, averaging 16% of the daily total in a recent review (Forster 2014). The failure to account for nighttime transpiration can lead to large underestimates throughout the day, due to misspecification of ΔT_0. Underestimation of daily transpiration from whole-tree chambers, where VPD exceeded ambient conditions, ranged from 70 to 98% depending on the degree of chamber heating and resulting VPD (Ward et al. 2008), when the effects of nighttime transpiration on ΔT_0 were not accounted for. Extrapolating this VPD relationship to ambient conditions suggested a ~30% underestimate outside of chambers, where VPD often failed to reach zero during the short summer nights of this high-latitude site.

Thus, consideration of how ΔT_0 is estimated is an important step of planning any study using TDPs, although the method employed is rarely reported in the resulting articles. Such reporting is especially important in large experiments with multiple sites and researchers (e.g., Will et al. 2015) to ensure that data are comparable across all experimental units. Likewise, in meta-analyses and large databases, variation in method of ΔT_0 determination is a potential source of bias when comparing data from different experiments.

TRACC software

Recognizing this need, we provide to the research community the TDP data processing software TRACC (Thermal dissipation Review Assessment Cleaning and Conversion) developed for use in the PINEMAP (http://www.pinemap.org) region-wide throughfall reduction and fertilization experiment (Will et al. 2015) in loblolly pine [*Pinus taeda* (L.)]. This software is a series of scripts in the language R (R Core Team 2016) which have been designed for users with little or no coding experience, with a series of user prompts that require simple yes/no or numeric answers (Fig. 1). R is a computing language made available under the GNU General Public License (GPL), Version 2, and thus should be free for all researchers to download and use (https://cran.r-project.org). Our scripts are provided via a public GitHub repository (https://github.com/ericward/TRACC) under the MIT License, allowing users with coding experience to suggest changes or extensions that others may find useful. They are not distributed as an R package, as we wanted those with no coding experience to be able to use them. The repository contains four R scripts, as well as the license (LICENSE.txt), an instruction file (README.txt), sample input (SampleFile.csv), and outputs (SampleClean.csv and SampleConv.csv).

The data required to run TRACC include the raw ΔT_M data and corresponding air temperature and vapor pressure deficit. Data can be collected at any time interval and the

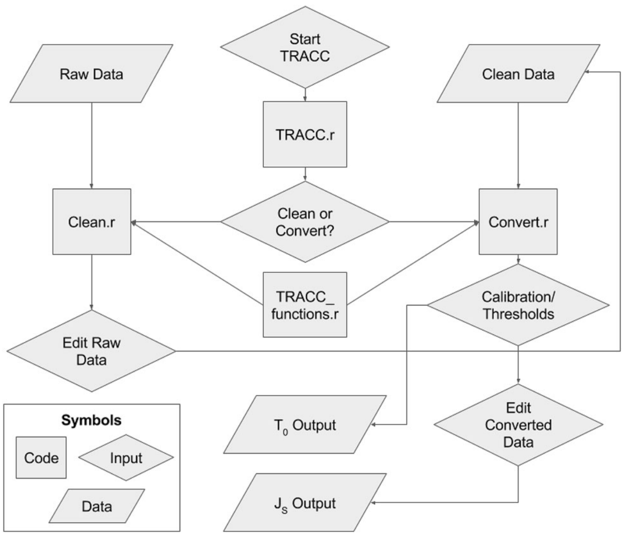

Fig. 1 Flowchart of TRACC software

number of sensors that can be handled will depend on the user's system. Testing on mid-range desktop computers has successfully run TRACC with over 100 sensors with a year of half-hourly data. As the ΔT_0 time series of each sensor is determined independently, the location of the sensor (individual tree, sensor depth, and aspect) is not needed. All sensors in a file will be evaluated based on a single air temperature and vapor pressure deficit time series, so sensors from sites that differ in these conditions need to be processed in separate files.

After installing R and formatting data according to the accompanying README file, the user simply places the data in the same directory as the four script files and runs the highest level script (TRACC.r) by typing a single line of code into the R console. All other interactions are handled by onscreen text prompts provided by the program. The first prompt asks the user to choose whether they want to clean or convert data. Depending on the answer, one of two other scripts (Clean.r and Convert.r) will be engaged. The last script (TRACC_functions.r) passes functions to the other scripts and contains most of the core calculations and data display functions. The required inputs and user-selected options for each process are summarized in Table 1.

If the user chooses to clean data, they then follow a series of text-based prompts to edit their raw ΔT_M data to produce a 'cleaned' data set. While this step depends on the user's own knowledge, it does ensure that the data from each TDP are inspected, first as a complete time series and then in a moving window with a user-specified width (defaulting to 2000 values). The user specifies upper and lower limits of acceptable ΔT_M values for both the data set as a whole at the beginning of the process, and for each sensor, once the entire data series for each has been visualized. These serve as coarse filters for erroneous measurements, which may be edited individually or across a range of time values as the data are presented in detail.

The output of this script can then be used as input for the conversion process, which uses similar text prompts to guide the user through determining appropriate ΔT_0 values. It then automatically linearly interpolates ΔT_0 values to form a continuous time series (referred to as a baseline) and converts ΔT_M to J_S values. The text prompts allow for user specification of not just the calibration coefficients α and β, but also defines a threshold of nights selected for determination of ΔT_0 in terms of a number of consecutive readings that must fall below a given VPD. A suggested value of four half-hourly readings at <0.1 kPa vapor pressure deficit is given in the instructions file (Ward et al. 2015), but the user is encouraged to use knowledge of the species and ecosystem studied to set these threshold parameters.

If this threshold is met on a given night, a ΔT_0 point is taken as the mean of the highest three readings before 5:30 AM on a given day at the time of the highest reading. This averaging reduces the impact of sensor noise on the baseline determination. These points are then interpolated across the data set to form the initial baseline assuming constant values before the first ΔT_0 point and after the final ΔT_0 point. After the initial baseline is placed, new ΔT_0 points are placed on nights where the mean nighttime reading is above the initial ΔT_0 time series between 2:00 and 6:00 AM, as the mean value of this period at 4:00 AM.

Table 1 Inputs and user selectable options for each process in TRACC

	Required inputs	User selectable options
Clean	1. Input 'raw' data filename	7. Window width for graphs
	2. Output 'clean' data filename	
	3. Upper limit for all sensors	
	4. Lower limit for all sensors	
	5. Upper limit for each sensor	
	6. Lower limit for each sensor	
Convert	1. Input 'clean' data filename	5. Window width for graphs
	2. Output 'converted' data and 'baseline' filenames	6. α and β values (Eq. 1)

These new ΔT_0 points are added to the initial ones and interpolated for the final baseline.

The effect of this threshold for determining nights with ΔT_0 on resulting sap flux density estimates is illustrated with sample PINEMAP data (Fig. 2). Applying this threshold over an entire year of data for 25 sensors resulted in a 7% increase in total sap flux when compared to using no threshold (i.e., assuming ΔT_0 was reached every night), with increases for individual sensors ranging from 2 to 16%. It should be noted that warm temperate forests, such as the one measured here, typically reach dew point during the night and have among the lowest percentages of nocturnal sap flow (Forster 2014). Results are likely to be more pronounced in continental, tropical, and boreal forests, as well as any experimental treatment that increases VPD (Ward et al. 2008). In addition, drought conditions characterized by high VPD at night may make sap flux estimates more sensitive to inaccurate estimates of $\Delta T_{0,}$ because these conditions may also induce low transpiration rates, i.e., small differences between ΔT_M and $\Delta T_{0.}$ (Eq. 2). Projections of future climates suggest that increasing VPD will be a significant constraint on the growth and transpiration of mesic forests (Novick et al. 2016) and a contributor of mortality in drier ones (McDowell et al. 2016).

Before the output is saved for each sensor, the final J_S values are presented to the user a final time for approval and editing. This script outputs the interpolated ΔT_0 values in a 'baseline' file as well as the converted values for archival purposes. Thus, when the user finishes the process, they will have four files that summarize the entire process for later review: the 'raw' input ΔT_M, the edited 'clean' ΔT_M, the 'baseline' of interpolated ΔT_0, and the final 'converted' J_S data. It is suggested that the user maintains all of these files for archival purposes. This not only helps maintain transparency of research, but may assist with retransforming data if, for example, it is later determined that different values of α and β are more appropriate.

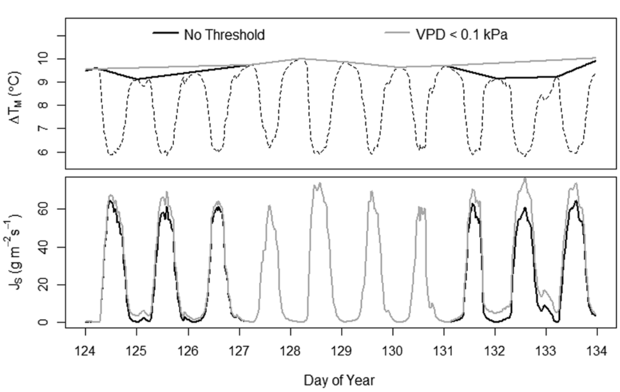

Fig. 2 (*Upper panel*) Temperature difference measured by probe (ΔT_M, *dashed*) and zero-flow difference (ΔT_0) estimated with (*gray*) and without (*black*) a nightly threshold of 0.1 kPa vapor pressure deficit for 2 h. (*Lower panel*) Resulting time series of sap flux density (J_S) using the two ΔT_0 estimates

Software platforms for TDP data

An advance offered by our open-source software is that it combines editing/conversion of (large) TDP data sets based on the experience and judgement of the user with automated data processing that rapidly corrects for potential systematic bias. Fully automating the processing of data from TDPs is made exceedingly difficult due to errors arising from many sources, including sensor failure, poor connectivity, thermal gradients in woody tissues, and degradation of thermal contact between the probe and sapwood (Lu e al. 2004). However, to the extent possible, it is desirable to minimize variation arising from different researchers processing data, and thus, a common platform for processing data, including editing raw data and determination of ΔT_0, is useful. This is not only true for researchers engaged in studies across multiple sites, but also studies conducted over multiple years at a single site, as personnel changes are common.

While commercially produced TDPs may be supplied with the appropriate software to provide such a common platform (e.g., ICT's Sap Flow Tool, http://www.sapflowtool.com/index.html), those that build their own sensors based on the original design (Granier 1985, Davis et al. 2012) require an open-source solution to this need. TRACC provides such an open-source solution. Another such program, BASELINER (Oishi et al. 2016), was recently released as both code for MATLAB (The MathWorks Inc., Natick, MA, USA) and a stand-alone Microsoft Windows executable. While this is available to a large audience, TRACC should be available to an even larger audience that includes those who do not have licenses for MATLAB on other operating systems and those who conduct other analyses in the R language. It should be noted that different software and methods of processing a ΔT_M data set will yield different results, depending on the assumptions made by the software or user. However, using a platform such as TRACC or BASELINER helps to ensure the replicability of results, should the impact of these assumptions need to be later evaluated.

Other software platforms are available for further processing and analyses of TDP data in the R language, including scaling from sensor to tree (Berdanier et al. 2016) and scaling from sensor to canopy conductance [STACC, (Bell et al. 2015)]. The outputs of TRACC could also easily incorporated into models constraining gross primary productivity estimates using TDP data [e.g., 4CA, (Schäfer et al. 2003)] and stand growth models that assimilate TDP data along with many other types of measurements [e.g., TREES, (Mackay et al. 2003, 2015)].

We have released this code publicly to encourage the research community using these techniques to exchange ideas and examine the assumptions that we use when we conduct experiments by expanding and building upon it. Future avenues for further development of this software by the community would include (1) making more aspects of baseline interpolation process user-configurable without overwhelming the beginner with too many choices, (2) more interactive graphical representations of data, and (3) metadata files that allow the user to save and load configurations of options. Open-source software such as TRACC and BASELINER can also serve as starting points for those developing software for related measurements, such as the processing of data collected with TDPs using newer, cyclical heating measurement schemes (Lubczynski et al. 2012; Reyes-Acosta et al. 2012), rather than the constant heating scheme of the original approach.

The ecophysiological community could benefit from more integrative platforms such as these, which also serve to increase the transparency of methodology, usefulness of archived data, and replicability of results (Ward 2016). In addition, adoption of a standardized TDP editing/conversion software platform would facilitate uniformity across large databases and long-term ecological monitoring networks such as SAPFLUXNET (http://sapfluxnet.creaf.cat/app), NEON (http://www.neonscience.org), LTER (https://lternet.edu), CZEN(http://www.czen.org), FLUXNET (https://fluxnet.ornl.gov), and ICOS (https://www.icos-ri.eu), to name a few.

Author contribution statement EJW conducted the analyses, authored the software, and drafted the manuscript. JCD and AN assisted with data collection, provided guidance on software development, and revised the manuscript. JK, GS, and SM provided critical revision of the article. All authors approved the final manuscript.

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Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

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