The Thellier Tool: A new software for analyzing absolute paleointensity determinations

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Abstract

The Thellier Tool is an intuitive and easy-to-use software which provides the possibility to analyze a wide range of different modifications of the Thellier absolute paleointensity experiment. Beside the Arai plot for paleointensity determination, orthogonal projections of the direction, decay of NRM during thermal demagnetization and additional plots regarding alteration and multidomain checks enable the user to visualize the quality of individual determinations. Experimental checks for magnetomineralogical changes, either in-field or zero-field pTRM* checks, are evaluated regarding their differences to the corresponding pTRM* acquisition in two most commonly used ways. Furthermore, a measure for the cumulative alteration differences beginning at room temperature is calculated and the possibility to correct for magnetomineralogical changes is provided. Two different experimental methods to check for multidomain bias are supported and analyzed by the software. Intensity differences recorded by pTRM*-tail checks are calculated. Accounting for the directional difference between applied laboratory field and NRM of the sample, the effective pTRM*-tail is determined and thus failures of Thellier's law of independence are monitored. Failures of the law of additivity, experimentally observed by additivity checks, are also evaluated by the software. The vector nature of individual measurements is fully considered for all calculations. Uniform selection criteria for acceptance and rejection of determinations can be applied and a set of such criteria with emphasize on minimal bias due to alteration, multidomain remanence and analysis inaccuracies are suggested.

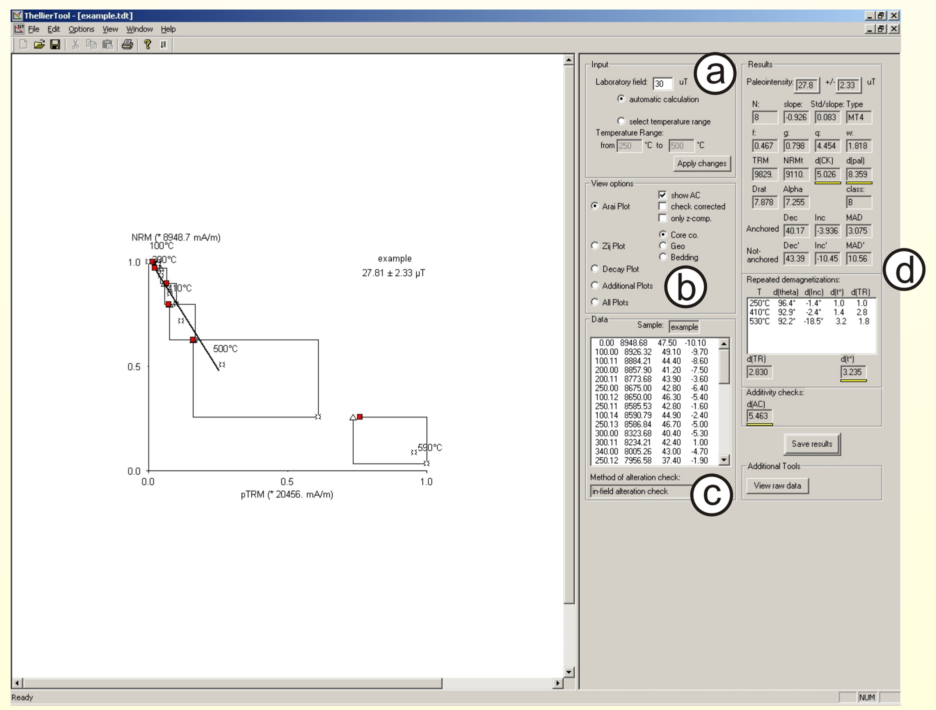


Fig. 2: The main window. The form view on the right side contains the results and several options regarding the data analysis. (a) contains the laboratory field and selected temperature interval. Four different view options are available (b), Arai plot, Zij plot, Decay diagram, and Additional plots. Raw data, as well as the used alteration check method are shown on the lower left of the form view (c). In inset (d) the obtained paleointensity value, as well as statistical parameters and other determination results are shown. The Save results button writes or appends all calculation results to a Tab-delimited text-file. The View raw data button opens the Thellier data file in Notepad.

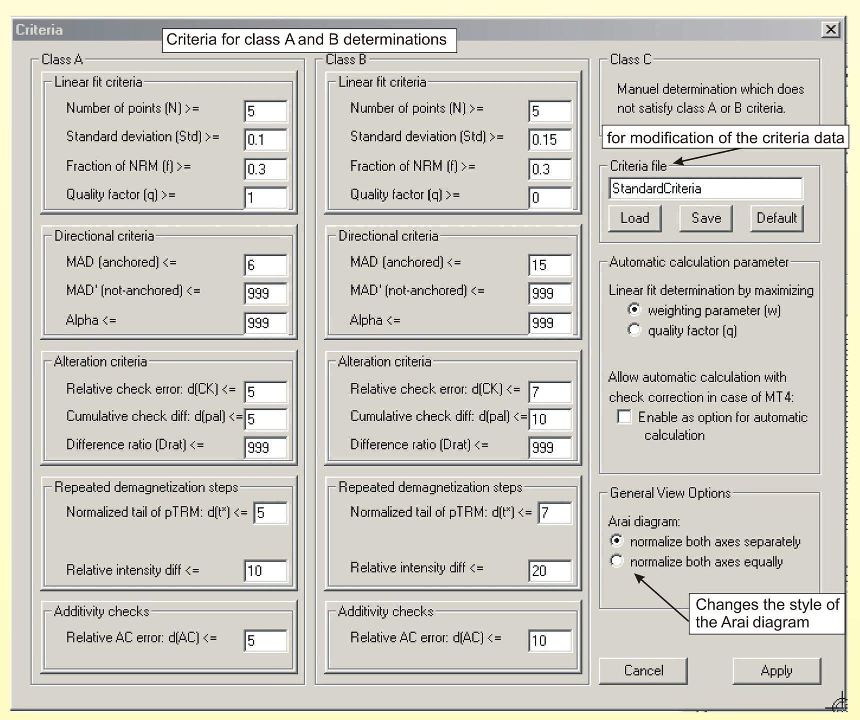


Fig. 4: The Criteria Dialog. Criteria, classifying the quality of the determination and the experimental checks can be specified in this dialog. It is possible to define a maximum of three different quality grades using specific criteria for classes A and B, as well as an authors choice C if at least one parameters exceeds class A and B criteria.

Data format, user interface and plots

Header (optional): laboratory field; geographic coordinates (bearing, plunge); bedding (direction of dip, dip)

Header (optional)	Thellier-tdt				
	25.000000	340.0	50.0	120.0	5.0
MGH1	20.00	4090,8	295.6	-42.8	NRM
MGH1	200.00	3734.2	302.4	-42.4	thermal demagnetization (TH)
MGH1	200.11	3972.4	303,0	-46.3	acqusition of pTRM (PT)
MGH1	200.13	3738.2	296.5	-42.6	pTRM*-tail check (TR)
MGH1	250.00	3617.1	300.2	-40.7	TH
MGH1	250.11	3303.9	300.2	-33.9	PT
MGH1	300.00	3447.4	297.4	-42.1	TH
MGH1	300.11	3918.4	293.8	-49.5	PT
MGH1	340.00	3284.2	297.9	-42.3	TH
MGH1	250.12	2984.2	293.1	-34.7	in-field pTRM*-check (CK)
MGH1	340.11	2796.1	295,0	-29.1	PT
MGH1	250.14	3059.2	296.5	-37.2	additivity check (AC)
MGH1	370.00	3146.1	297.1	-42,0	TH
MGH1	370.11	3811.8	298.7	-51.8	PT
MGH1	370.13	3143.4	298.2	-42,0	TR
MGH1	400.00	3042.1	298.6	-41.9	TH
MGH1	340.12	2598.7	298.2	-27.4	CK
MGH1	400.11	2486.8	296.9	-23.2	PT
MGH1	340.14	2886.8	300.6	-38.3	AC
...	...	...	...	...	...

(Data)

Fig. 1: Example input file format of a zero-field first, in-field alteration check Thellier experiment. The data of the Thellier measurement is given in 5 columns: Column 1 contains the sample name (maximum length of 16 characters), column 2 the temperature (in °C) and type of measurement, column 3 the intensity (in mA/m), column 4 the declination and column 5 the inclination in core coordinates. The decimal digits of the temperature value (column 2) indicate the type of measurement: .00 (or .0) stands for thermal demagnetization, .11 (or .1) denotes pTRM* acquisition, .12 (or .2) defines the pTRM*-check, .13 (or .3) repeated demagnetization steps and .14 (or .4) indicates additivity checks.

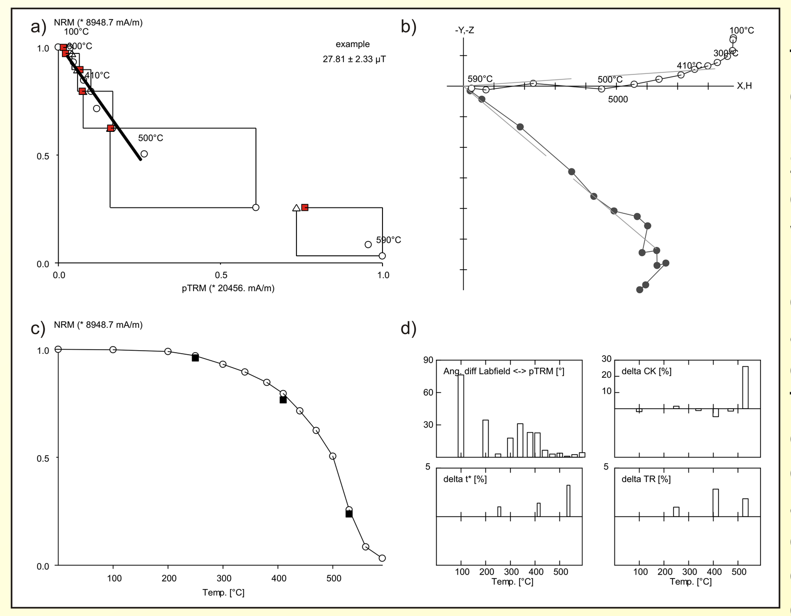


Fig. 3: Available plots of the ThellierTool. (a) the NRM/TRM diagram, (b) the orthogonal projection of the demagnetization data, (c) the decay diagram and (d) additional plots, which are the difference between the applied field direction and the direction of the acquired pTRM*, the individual check errors normalized to the TRM, the tail of the pTRM* corrected for the angular difference between applied field and NRM, and the intensity difference between first demagnetization and repeated demagnetization.

Correcting magnetomineralogical changes

If alteration checks are continuously and subsequently performed over the entire experimental temperature range and assuming that alteration happens predominantly below the temperature of the respective check, a method can be used to correct for magnetomineralogical changes during laboratory treatment (Valet et al., 1996; Leonhardt et al., 2003). For this technique, the cumulative sum of the individual differences between checks and associated pTRM* values up to heating step i-1 is subtracted from the measured pTRM* value at step i. Such correction is conducted by selecting the view option **check corrected** (Figure 2b), resulting in a recalculation of pTRM*-acquisition values and all dependent vector subtractions. The class is extended by a star (e.g. A*) if check correction is selected. A further fundamental requisite for this correction method is the absence of MD remanence, since such remanence biases also the pTRM*-checks used for cumulative difference calculations (Leonhardt et al., in press).

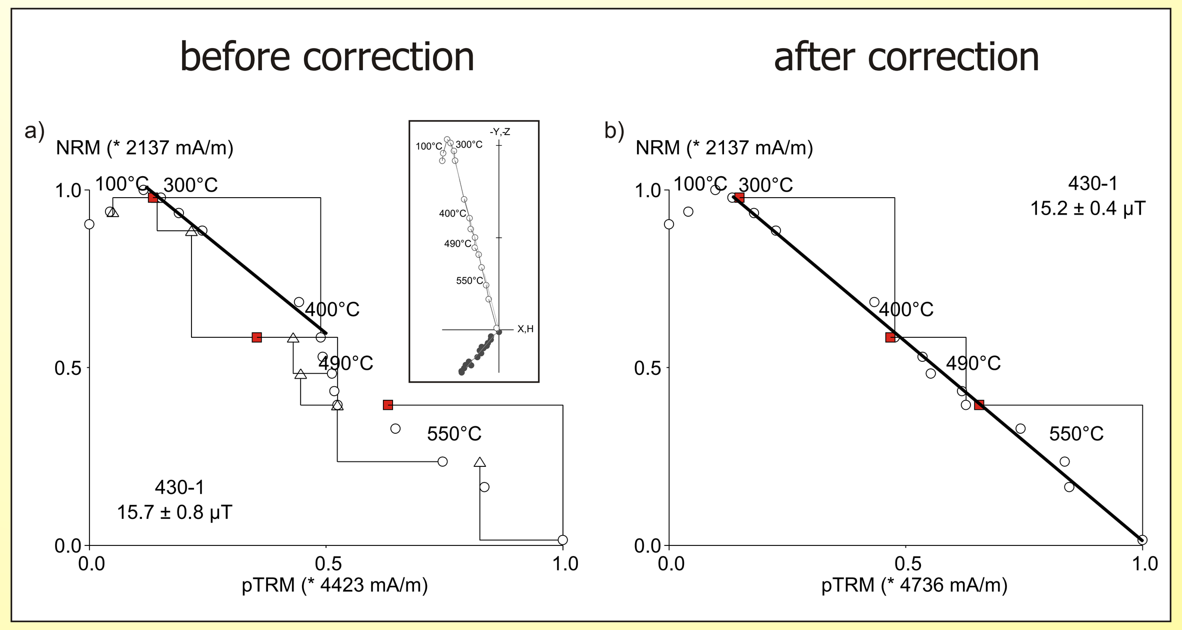


Fig. 5: In (a) magnetomineralogical changes above 400°C are present as indicated by deviating pTRM*-checks. The repeated demagnetization steps show no significant influence of MD remanence for this example. After check correction, the additivity checks coincide with the pTRM* values indicating successful correction and a linear segment covering most of the blocking temperature spectrum is obtained. Note that similar intensities are obtained in (a) and (b).

Per default all calculations are done using full vector subtraction. If view option **z-comp only** (Figure 2b) is selected, the vector subtraction is done by using only the values for the measured z-component (in core coordinates), requiring that the applied field is parallel to the core coordinate z-component of the sample. All parameters are then recalculated.

Detecting multidomain bias

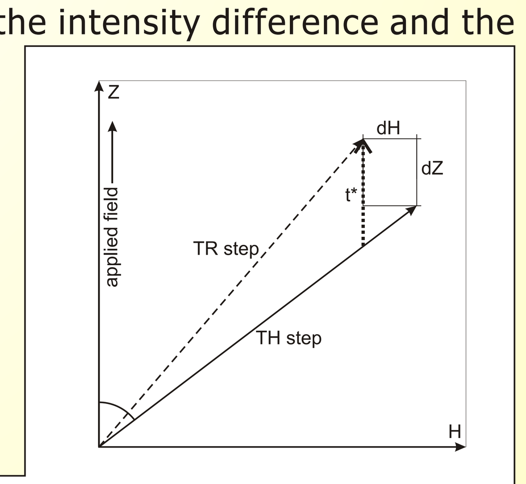
When employing the Thellier method for paleointensity determination, the pTRM is acquired by heating a sample to T_i with $T_i < T_C$ and applying a laboratory field during cooling from T_i to T_0 (pTRM*). Significant differences between pTRM* and pTRM, where T_i is reached by cooling from T_C, are observed (Shcherbakov et al., 1993). This discrepancy leads to failures of Thellier's laws of independence and additivity, which are only fulfilled for magnetic grains showing single domain (SD) character and, therefore, an equality between unblocking (T_{ub}) and blocking (T_b) temperatures. Checks for failures of both laws are supported by the ThellierTool.

Independency check

The tail of the pTRM* leads to an acquisition of remanence for $T_{ub} > T_b$. The curvature in the Arai diagram, as well as the alteration checks and the pTRM*-tail checks are affected by the intensity difference and the directional difference between the natural ambient field and the laboratory field (Leonhardt et al., in press). According to the phenomenological model of Leonhardt et al. (in press), the high-T tail can be estimated by:

$$t^* = |H_N/H_{lab}\ (dZ - dH/\tan\quad)|$$

as long as > 0. d(t*) is calculated by normalizing t* to NRMt (Fig. 6).



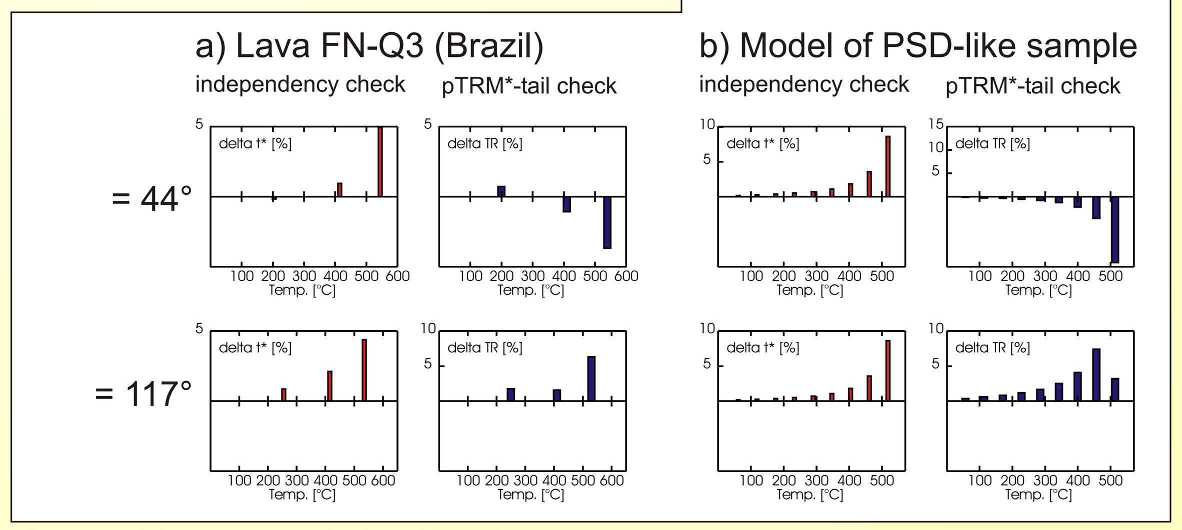


Fig. 6: (a) Vectors of the first demagnetization step (TH-step) and the repeated demagnetization step (TR-step) which is affected by a pTRM*-tail (t*). The laboratory field is applied along the z-axis. Due to the tail, the repeated magnetization differs by dZ (= $z_{TH} - z_{TR}$) and dH (= $\sqrt{(x_{TH}^2 + y_{TH}^2)} - \sqrt{(x_{TR}^2 + y_{TR}^2)}$) from the original vector, where x, y, z are the remanence components in sample coordinates of the TH and TR step. denotes the angle between applied field and the remaining NRM of the first demagnetization step. In (b) and (c) comparisons of pTRM*-tail checks (Riisager et al., 2001) and directional corrected tail checks (independency checks) are shown. For Thellier determinations from lava flow FN-Q3 (Leonhardt et al., 2003) and a PSD-like model (Leonhardt et al., in press), d(t*) gives similar values for two different , whereas the pTRM*-tail check gives different values. Positive d(t*) values indicate an acquisition of a tail in direction of the applied field. Negative values cannot be related to tails and point rather to alteration or stabilization processes during repeated heating steps affecting temperature ranges above the actual heating step.

Additivity check

For the additivity check (Krása et al., 2003) a pTRM*(T_0,T_i) is subsequently demagnetized to T_k ($T_k < T_i$). Vector subtraction is then conducted between these measurements without prior isolation of the pTRM*. Using this technique, any previous tail bias is subtracted as well. This additivity check value can then be compared to the isolated pTRM*(T_0,T_k). Thus, the measurement as well as the calculation are evidently the same as for zero-field pTRM*-checks. Due to the added sensitivity to remanences with $T_{ub} < T_b$ of the additivity check a comparison of in-field pTRM*-checks and additivity checks enables one to recognize failures of Thellier's law of additivity.

Calculated parameters

- ***N***: number of succesive points in linear segment.
- ***std/slope***: standard deviation versus slope of linear segment.
- ***f, g, q***: fraction of NRM (f), gap factor (g), quality factor (q) are calculated according to Coe (1978).
- ***w***: weighting factor (w) of Prévot et al. (1985).
- ***NRMt***: The "true" NRM (NRMt) is the intersection between linear fit and y-axis.
- ***TRM***: the intersection between linear fit and x-axis.
- ***Inc, Dec, MAD***: Inclination, Declination, and maximum angular deviation for an origin-anchored line fit of first demagnetization steps (using principle component analysis).
- ***Inc', Dec', MAD'***: non-anchored directional results.
- ***alpha***: angular difference between anchored and not-anchored solution.
- ***class***: quality grade assigned by determination criteria.
- ***type***:
  MT0: Thellier-type method without any checks
  MT1: "Field-off first" method with pTRM*-checks
  MT2: "Field-on first" method with pTRM*-checks
  MT3: Method MT1 including pTRM*-tail checks
  MT4: Method MT1 including pTRM*-tail checks and additivity checks
- ***d(CK)***: the difference between pTRM*-check and related pTRM* acquisition, normalized to ***TRM***
- ***DRAT***: like ***d(CK)*** but normalized to the length of the selected segment (Selkin and Tauxe, 2000)
- ***d(pal)***: cumulative check error, related to the cumulative difference of the individual checks from room temperature up to the maximum temperature used for the selected linear segment. The correction method for magnetomineralogical changes which uses the cumulative sum of alteration differences is applied to the selected segment and the check corrected paleointensity value is compared to the non-corrected value. ***d(pal)*** is the ratio of uncorrected to corrected paleointensity normalized to the uncorrected value.
- ***d(TR)***: intensity difference of first and repeated demagnetization step normalized to ***NRMt***.
- ***d(t*)***: relative extend of the "true" tail according to Leonhardt et al. 2004.
- ***d(theta)***: angle between applied field and NRM of the sample
- ***d(Inc)***: inclination difference of first and repeated demagnetization step.
- ***d(AC)***: difference between additivity check and related pTRM* acquisition, normalized to ***TRM***.

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