

Low-T Thermo: a new program for arbitrarily combining low-T thermochronological data to model thermal history

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Abstract

A robust code, designated Low-T Thermo, has been developed to arbitrarily combine low-T thermochronological data for thermal history modeling. With the development of methods that treat apatite fission-track age and confined length as two completely independent datasets for thermal history inversion, and those employing mica Ar-Ar age or bedrock quartz optically stimulated luminescence age for thermal history inversion, eight types of low-T thermochronological data are now available for thermal history modeling: apatite fission-track age, apatite fission-track confined length, zircon fission-track age, apatite (U-Th)/He age, zircon (U-Th)/He age, mica Ar-Ar, bedrock quartz optically stimulated luminescence age, and vitrinite reflectance. In theory, a total of 247 combination modes can be employed for joint thermal history inversion (excluding the eight single-method modeling approaches). These arbitrary combinations facilitate thermal history modeling using “incomplete” low-T thermochronological datasets that would otherwise be considered unusable for thermal history modeling, thereby reducing experimental costs. For arbitrary combinations of different low-T thermochronological data, each method exhibits incomplete independence, and the equivalent p-value serves as the uniform evaluation metric in the inversion process. The utility of the code is demonstrated through thermal history modeling of existing low-T thermochronological data from the Dabie Mountain, Ahimanawa Range, and Southern Alps regions.

Full Text

Preamble

Low-T Thermo: A New Program for Arbitrarily Combining Low-Temperature Thermochronological Data to Model Thermal History

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Abstract: A robust code called Low-T Thermo has been developed to arbitrarily combine low-temperature thermochronological data for thermal history modeling. Following the decoupling of apatite fission-track age and confined length into two completely independent datasets for thermal history inversion, and with the development of thermal history inversion using mica Ar-Ar age or bedrock quartz optically stimulated luminescence age, there are now eight types of low-temperature thermochronological data used to invert thermal history: apatite fission-track age, apatite fission-track confined length, zircon fission-track age, apatite (U-Th)/He age, zircon (U-Th)/He age, mica Ar-Ar age, bedrock quartz optically stimulated luminescence age, and vitrinite reflectance. A total of 247 combination modes are theoretically available for jointly inverting thermal history (excluding the eight single-method approaches). These arbitrary combinations facilitate thermal history modeling using “incomplete” low-temperature thermochronological datasets previously considered unusable for thermal history modeling, thereby reducing experimental costs. For arbitrary combinations of different low-temperature thermochronological data, each method is not completely independent, and an equivalent p-value serves as the uniform evaluation metric in the inversion process.

The utility of the code is demonstrated by modeling thermal histories from existing low-temperature thermochronological data in the Dabie Mountains, Ahi-manawa Range, and Southern Alps.

Keywords: Low-T Thermo; Thermal history modeling; Low-temperature thermochronology

1 Introduction

Low-temperature thermochronology (including apatite and zircon fission-track analysis, (U-Th)/He dating, and $^{40}\text{Ar}/^{39}\text{Ar}$ dating) is a widely used tool for investigating tectonic and surface processes, providing quantitative thermal history information for rock samples. Over the years, numerous increasingly sophisticated programs have been developed to extract thermal histories from low-temperature thermochronological data (e.g., Corrigan, 1991; Gallagher, 1995; Willett, 1997; Ketcham et al., 2000; Ketcham et al., 2005; Gallagher, 2012). Beyond using apatite fission-track data alone, various combinations of different low-temperature thermochronological methods have been employed for joint thermal history inversion (Ketcham, 2005). For example, (U-Th)/He and fission-track data have been combined to invert thermal history directly, rather than using

(U-Th)/He age merely as a constraint box for fission-track inversion. However, the available combination modes have been very limited.

Here we present a new program for modeling thermal history from low-temperature thermochronology. This program can arbitrarily combine eight types of low-temperature thermochronological data for joint thermal history inversion: AFT age, AFT confined length, zircon fission-track (ZFT) age, apatite (U-Th)/He age (AHe), zircon (U-Th)/He age (ZHe), mica Ar-Ar age, optically stimulated luminescence (OSL) age of bedrock quartz, and vitrinite reflectance (Ro). AFT age and confined length are decoupled into two completely independent datasets (Ding, 2017). Additionally, mica Ar-Ar and bedrock quartz OSL ages are incorporated for thermal history modeling. Consequently, 247 combination modes are theoretically available (excluding the eight single-method approaches), irrespective of local geological constraints. These arbitrary combinations facilitate thermal history modeling using “incomplete” datasets previously considered unusable for thermal history modeling, thereby reducing experimental costs.

The program is designed for ease of use by non-specialists. It is available free of charge for academic and non-profit research by contacting the author. Operating instructions and update information are provided on the website: <http://low-T.me>.

2.1 Forward Modelling

In the forward modeling procedure, the thermal history is first discretized into 100 evenly spaced time steps (except for OSL, which uses a 1 ka time step), after which it is converted into modeled ages or reduced length distributions of confined tracks.

Apatite Fission-Track Age and Confined Length: The fanning curvilinear annealing model of Ketcham et al. (2007) is used for C-axis projected track lengths, assuming an rnr_0 value of 0.83. The equation for fission-track length for C-axis projected track lengths follows Ketcham et al. (2007). The initial C-axis projected track length is 16.62 μm (Ketcham et al., 2009). A minimum detectable length of 7.31 μm is assumed for C-axis projected track lengths (Donelick et al., 1999). The relationship between C-axis projected length and standard deviation is obtained by fitting data from Carlson et al. (1999) based on the projection model of Ketcham (2007) (Appendix: Ketcham et al., 2007). Modeled fission-track dates are calculated by dividing the cumulative track density at each time step by 0.893 (Ketcham et al., 2000). The conversion model from fission-track length to density presented by Donelick et al. (1999) is employed. The Kolmogorov-Smirnov (K-S) test probability (i.e., p-value; Marsaglia et al., 2003) is calculated based on the C-axis projected confined track-length distribution. Forward-modeled AFT ages and length distributions are statistically consistent with HeFTy (Ketcham, 2005).

Zircon Fission-Track Age: The annealing model formula is $1/\ln(1/0.05721$

Guenther et al. (2013). The relation $\rho = \rho_0 \exp(-r/\lambda)$ (Tagami et al., 1990; Guenther et al., 2013) is used to convert reduced length (r) to reduced density (ρ). KT06 zircon can be used as an age standard for calibration, with unannealed spontaneous track lengths of 10.89 μm and induced track lengths of 10.94 μm (Tagami et al., 1990). The ratio of spontaneous to induced track length in the standard is therefore 0.995. Because this ratio is close to 1, it can also be set to 1.

Apatite and Zircon (U-Th)/He: The spherical diffusion equation (Carslaw and Jaeger, 1959), Arrhenius formula, (U-Th)/He age calculation formula (Farley, 2002), and radiation damage accumulation and annealing models for apatite (RDAAM: Flowers et al., 2009) and zircon (ZrRDAAM: Guenther et al., 2013) are used to represent the relationship between (U-Th)/He age and thermal history. For (U-Th)/He, the alpha stopping distance can be defined following Farley et al. (1996) or Ketcham et al. (2011). The finite difference method (Ketcham, 2005) is used to calculate modeled (U-Th)/He ages from the thermal history. Forward-modeled AHe ages are statistically concordant with those calculated by HeFTy (Ketcham, 2005).

Vitrinite Reflectance: Low-T Thermo currently includes three vitrinite reflectance calibrations: the widely used EASY %Ro method of Sweeney and Burnham (1990), the “IKU” calibration described by Ritter et al. (1996), and the “basin %Ro” calibration of Nielsen et al. (2016). Low-T Thermo initiates Ro value calculations from the given depositional age (Stratigraphic Age) of the sample, assuming that Ro values form after deposition. If the Stratigraphic Age exceeds the modeling duration or is not provided, the modeling duration is used as the Stratigraphic Age.

Bedrock Quartz OSL: Following Herman et al. (2010), the formula describing accumulation of trapped electrons with decreasing temperature $n = N \exp(-E_a/RT) [1 - \exp(-P \cdot t)]$ (Randall and Wilkins, 1945) is used, where N is the number of trapped electrons, t is time (a), E_a is activation energy (J/mol), $0D$ is the frequency factor (m^2/s) in the Arrhenian expression of the diffusion coefficient, R is the gas constant (8.3145 J/(mol · K)), T is absolute temperature (K), P is a filling rate (a^{-1}), and $Asat$ is the saturation age (a). The finite difference method is used to calculate modeled OSL ages from the thermal history.

Mica Ar-Ar: The spherical diffusion equation (Carslaw and Jaeger, 1959) is used to represent the relationship between Ar-Ar age and thermal history, without considering pressure effects, etc. The sphere radius is calculated using the closure temperature expression given by Dodson (1973): $r = \sqrt{A \cdot cT / \dot{T}}$, where r is the sphere radius (m), A is a geometric factor (55 for a sphere), cT is the closure temperature (K), and \dot{T} is the cooling rate ($^{\circ}\text{C}/\text{Ma}$). Once the mica Ar-Ar closure temperature is assumed for a given cooling rate, the sphere radius can be calculated, after which the finite difference method is used to solve the diffusion equation. In Low-T Thermo v1.0, after specifying the widely accepted closure temperature range at a cooling rate of 10 $^{\circ}\text{C}/\text{Ma}$, a corresponding age range can be calculated. Therefore, for a given thermal history, the modeled result is an

age range.

2.2 Inverse Modelling

In this inverse process, we use the Monte Carlo method to randomly search through thermal histories (e.g., 10,000 paths) in which time-temperature points are not regularly distributed and can be randomly perturbed.

To compare different methods, the p-value is used as a uniform metric to evaluate misfit. For apatite fission-track lengths, the p-value is derived from a K-S test. For ages, equivalent p-values are calculated assuming a normal distribution: $p = \frac{O - M}{\sigma}$, where O is the measured age, M is the modeled age, and σ is the standard deviation of the measured age. A 1 age standard deviation is equivalent to a K-S test p-value of 0.32. When different methods are combined, the minimum p-value among all methods is used as the final result.

The mean thermal history is calculated from all paths that meet a threshold equivalent p-value, which serves as the modeling result. The threshold equivalent p-value, i.e., the acceptable goodness-of-fit (GOF), can be set to 0.5, 0.32, 0.05, etc., depending on the dataset. Because time-step sizes are variable, each selected thermal history is resampled into 100 evenly spaced time steps to calculate the mean temperature at each node.

For multiple (U-Th)/He grain ages, the “Using multiple ages” option inverts each grain individually, while the “Using mean age” option performs inversion using the mean age of multiple grains with error propagation. When using this option, the helium content and its error for each grain are calculated from the ^{23}U , ^{235}U , and ^{232}Th contents and their errors using the age calculation formula (Farley, 2002). The mean ^{23}U , ^{235}U , ^{232}Th , and He contents and their errors are then used to calculate the mean (U-Th)/He age and its error.

Because the OSL method requires more accurate modeling than other methods for the time interval between 0 and 0.5-1 million years, at least one constraint box within 0-1 million years is required. Additionally, when bedrock quartz OSL is selected, the “Duration” parameter should ideally be of single-digit magnitude (<10 Ma), with smaller values being preferable.

The mica Ar-Ar method uses a modeled age range as its result, and the measured age within the acceptable GOF is also considered a range. Therefore, if these two ranges overlap, the assumed thermal history is considered acceptable.

3 General Workflow

Low-T Thermo is written for the Microsoft Windows operating system, primarily using Mathematica. Therefore, Mathematica 8 or 9 must first be installed, and the Wolfram.NETLink.dll file must be copied into the same directory as the main program (Low.exe). Additionally, Microsoft .NET Framework 2.0 must also be installed.

The workflow within Low-T Thermo is illustrated in Fig. 1 [Figure 1: see original paper]. Users first select the desired low-temperature thermochronological methods, then input the corresponding data (e.g., ages) via simple copy-and-paste operations. Required parameters include surface temperature at sea level, elevation, atmospheric lapse rate, maximum temperature for the temperature axis, maximum time for the time axis, number of paths attempted during inversion, acceptable GOF threshold, and geological constraint boxes.

After modeling, the results display the modeled thermal history and modeled ages or values for each selected low-temperature thermochronological method. The “Modeled AFT Length Distribution” form displays the AFT confined track length distribution. The “Modeled He Age Distribution” form shows the He age distribution as a function of effective uranium concentration (eU), based on the radiation damage accumulation and annealing models for apatite (RDAAM: Flowers et al., 2009) and zircon (ZrRDAAM: Guenther et al., 2013).

All output graphs and data can be exported to the working directory. Graphs are saved as PDF files that can be edited in various graphics packages, such as Adobe Illustrator and CorelDRAW.

Fig 1. Flow chart describing various input options and parameters of Low-T Thermo as well as output fields.

3 Real Examples

We now present examples to test various data combinations. Test cases include sample DB40 from Reiners et al. (2003) and Zhou et al. (2003), sample JR11-08 from Jiao et al. (2014), and mean age values from Southern Alps samples (MSA) (Herman et al., 2009, 2010). The present-day surface temperature is calculated as $T_s = T_0 - \gamma \times h$, where T_0 is the surface temperature at sea level, γ is the atmospheric lapse rate, and h is the elevation.

Example 1: DB40 is located at Tiantangzhai peak in the Dabie Mountains, China, which experienced rapid exhumation during the Late Cretaceous. For this modeling test, AFT age, ZFT age, and biotite $^{40}\text{Ar}/^{39}\text{Ar}$ age data for DB40 are used to model the thermal history. The age data are shown in Table 1. T_0 is 15 °C and γ is assumed to be 6 °C/km. The ratio of ZFT spontaneous to induced track length in the standard is set to 1. The closure temperature of biotite $^{40}\text{Ar}/^{39}\text{Ar}$ age is 350–400 °C for a cooling rate of 10 °C/Ma (Grove and Harrison, 1996; Harrison et al., 1985). Activation energy is 210 kJ/mol and the frequency factor is 0.40 cm²/s (Grove and Harrison, 1996).

In this inverse process, 10,000 thermal histories were randomly searched. The thermal history modeling result is shown in Fig. 2 [Figure 2: see original paper]. The resulting models are very similar to those determined by Zhou et al. (2003) based on both AFT age and confined length using AFTSolve software (Ketcham et al., 2000).

Table 1. The age data of DB40 Sample Elevation AFT age ZFT age $^{40}\text{Ar}/^{39}\text{Ar}$

age Note: AFT age and ZFT age of DB40 are from Reiners et al. (2003) and Zhou et al. (2003), and biotite $\text{Ar}/^3\text{Ar}$ age is plateau age from Chen et al. (1995).

Fig 2. Model result of AFT age + ZFT age + biotite $\text{Ar}/^3\text{Ar}$ age of DB40 in Dabie Mountain, China. 10,000 thermal histories are used for the Monte Carlo random search. The green range is more than Acceptable Fit. The pink range is more than high GOF (0.5). The black line, the mean history of all paths with high GOF (0.5) is as modeled result. The corresponding modeled age results are also shown in textboxes.

Example 2: JR12-14 is from the Ahimanawa Range in the central North Island, New Zealand, where basement rocks were exhumed to shallow crustal depths in the Early Cretaceous, subsequently reheated, and then exhumed to shallow depths again. For this modeling test, AFT confined lengths and AHe ages of JR12-14 are used to model the thermal history. The age data are shown in Table 2. T_s is 11 °C and β is assumed to be 5 °C/km.

In this inverse process, 100,000 thermal histories were randomly searched. The thermal history modeling result is shown in Fig. 3a [Figure 3: see original paper]. The resulting models are similar to those of Jiao et al. (2014), obtained using QtQt software (Gallagher, 2012) based on AFT data (both ages and confined lengths) and AHe ages from a vertical profile. However, it should be noted that QtQt does not require constraint boxes, whereas Low-T Thermo requires them for reheating modeling. The modeled He age distribution (Fig. 3b) shows the He age distributions for two grains as a function of eU.

Table 2. AHe data and AFT length data of JR12-14 Sample Elevation Grain (ppm) (ppm) AHe age length JR12-14 Note: JR12-14 is from Jiao et al. (2014).

Fig. 3 The thermal history modelling using different AHe grain-age data and confined track lengths (AHe age + AFT length) of JR12-14 in Ahimanawa Range, New Zealand. a) JR12-14 thermal history modelling based on combining three AHe grain ages and the AFT confined track lengths. All the thermal histories have 0.05 p-values. 100,000 thermal histories are used for the Monte Carlo random search. The minimum equivalent p-values is taken as the evaluating parameter. The green range is more than Acceptable Fit. The pink range is more than high GOF (0.5). The black line, the mean history of all paths with high GOF (0.5) is as modeled result. The corresponding modeled age results are also shown in textboxes. b) The corresponding modeled He age distribution with eU according RDAAM (Flowers et al, 2009) and AFT length distribution.

Example 3: Samples from the central Southern Alps of New Zealand experienced cyclic glaciations that began in the Pliocene around 2.5 ± 0.1 Ma (Suggate, 1990) and an extreme exhumation event occurred at 0.1 Ma (Herman et al., 2010). For this modeling test, AHe ages, ZHe ages, and bedrock quartz OSL ages from MSA are used to model the thermal history. The age data are shown in Table 3. T_s and β are the same as in Example 2.

In this inverse process, 100,000 thermal histories were randomly searched. A constraint box from 0.1 to 0.5 Ma is used. The thermal history modeling result is shown in Fig. 4 [Figure 4: see original paper]. The resulting models are highly concordant with those estimated by Herman et al. (2010).

Table 3. AHe, ZHe and Bedrock Quartz OSL age of MSA Sample Elevation (ppm) (ppm) AHe age ZHe age total dose Equivalent OSL age rate (mGy/a) dose (Gy) Note: All of the data are the mean value of samples in Southern Alps (Herman et al., 2009; 2010)

Fig 4. Model result of mean AHe age + ZHe age + Bedrock Quartz OSL age of the samples in Southern Alps, New Zealand. 100,000 thermal histories are used for the Monte Carlo random search. The green range is more than Acceptable Fit. The pink range is more than high GOF (0.5). The black line, the mean history of all paths with high GOF (0.5) is as modeled result. The corresponding modeled age results are also shown in textboxes.

4 Conclusions

A new, user-friendly code called Low-T Thermo has been developed to arbitrarily combine low-temperature thermochronological data for thermal history modeling. These data include AFT age, AFT confined length, ZFT age, AHe age, ZHe age, Ro, mica Ar-Ar age, and bedrock quartz OSL age. These methods are not completely independent. Although different combinations offer different advantages for thermal history modeling—because each low-temperature thermochronological method has its own strengths in constraining thermal evolution—these arbitrary combinations are particularly useful for modeling thermal histories from “incomplete” low-temperature thermochronological datasets previously considered unusable, thereby reducing experimental costs.

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