

Computational Tools for Low-Temperature Thermochronometer Interpretation

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INTRODUCTION

This volume highlights several applications of thermochronology to different geologic settings, as well as modern techniques for modeling thermochronometer data. Geologic interpretations of thermochronometer data are greatly enhanced by quantitative analysis of the data (e.g., track length distributions, noble gas concentrations, etc.), and/or consideration of the thermal field samples cooled through. Unfortunately, the computational tools required for a rigorous analysis and interpretation of the data are often developed and used by individual labs, but rarely distributed to the general public. One reason for this is the lack of a good

medium to communicate recent software developments, and/or incomplete documentation and development of user-friendly codes worth distributing outside individual labs. The purpose of this chapter is to highlight several user-friendly computer programs that aid in the simulation and interpretation of thermochronometer data and crustal thermal fields. Most of the software presented here is suitable for both teaching and research purposes.

Table 1 summarizes the different programs discussed in this chapter, the contributing authors behind each program¹, the computer operating system each program runs on, and the application or purpose each program is intended for simulating. The intent of this chapter is not to provide a user manual for each program, but rather an introduction to concepts and physical processes each program simulates. All software discussed here is freely available for non-profit applications and can be downloaded from <http://www.minsocam.org/MSA/RIM/> under the link for Volume 58, *Low-Temperature Thermochronology*. This web page contains executable versions of the software, copyright information, example input and output data files, and, in some cases, additional documentation and user manuals. The availability of source code for modifying each program varies, and interested persons are encouraged to contact the leading contributor. Regular users of these programs are encouraged to contact the software contributor to receive software updates and bug fixes. Software updates will occasionally be posted on the MSA web server as well. Software users should be aware of the caveats associated with use of these programs².

The remainder of this chapter is dedicated to highlighting the functionality of each software package. Several items are discussed for each software package. These items include: (1) the intended application of each program and motivation behind its development, (2) the general theory and equations solved in the program, (3) the input required to run the program, and (3) the output generated.

TERRA: FORWARD MODELING EXHUMATION HISTORIES AND THERMOCHRONOMETER AGES

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The TERRA (Thermochronometer Exhumation Record Recovery Analysis) software simulates rock thermal histories and thermochronometer ages generated during exhumation. There are two linked modules to this program. The “Thermal Calculation” module calculates cooling histories for either 1D transient heat transfer with variable erosion rates, or 2D steady-

¹ **Suggested format for referencing software described in this chapter:** Each computer program described in this chapter was developed by different contributors (Table 1). To assure each contributor receives appropriate credit for their contribution please include the contributor and software names in any citations used in publications. For example, programs in this volume could be cited in the following way, “We computed erosion rates using the program AGE2EDOT developed by M. Brandon and summarized in Ehlers et al. (2005).” If additional publications are available describing the software (e.g., HeFTy; Ketchum et al. 2005) please also reference those publications.

² **Caveats related to software use and distribution:** There are two caveats associated with the software provided in this volume. (1) The software is provided as a courtesy to the broader scientific community and in some cases represents years of effort by the contributors. The software can be used free of charge for non-profit research, but persons with commercial or for-profit interests and applications should contact the contributors concerning the legalities of its use. (2) Although every effort has been made by the contributors to assure the software provided functions properly and is free of errors, no guarantee of the validity of the software and results calculated can be made. Thus, application of the software is done at the users own risk and the software contributors are not accountable for the results calculated.

Table 1. Summary of software contributions.

<i>Program Name</i>	<i>Contributors</i>	<i>Application / Purpose</i>	<i>Operating Systems Supported</i>
TERRA	T. Ehlers, T. Chaudhri, S. Kumar, C. Fuller, S. Willett	Forward modeling thermochronometer ages, apatite and zircon fission track and (U-Th)/He	Windows [®] , Linux
HeFTy	R. Ketcham	Forward and inverse modeling apatite fission track, (U-Th)/He, vitrinite reflectance data	Windows [®]
BINOMFIT	M. Brandon	Calculate ages and uncertainties for concordant and mixed distributions of FT grain ages	Windows [®]
CLOSURE, AGE2EDOT, RESPTIME	M. Brandon	Calculate effective closure temperatures, erosion rates, and isotherm displacement for several thermochronometer systems	Windows [®]
FTIndex	R. Ketcham	Calculated index temperatures and lengths of fission track annealing models	Windows [®]
TASC	D. Belton, B. Kohn, A. Gleadow	Fission track age spectrum calculations	Windows [®] (Excel [®])
DECOMP	T. Dunai	Forward modeling (U-Th)/He age evolution curves	Windows [®]
4DTHERM	F. Fu	Thermal and exhumation history of intrusions	Windows [®] , Linux, Mac [®]

state heat transfer for user defined periodic topography and erosion rates. The “Age Prediction” module uses the thermal histories generated in the first module, or any other user defined thermal histories, to calculate cooling rate dependent apatite and zircon (U-Th)/He ages, and apatite and zircon fission track ages. The program is platform independent and runs on Windows[®] XP, and Linux[®] operating systems. Future releases of the program will run on the Macintosh[®] operating system as well. A graphical user interface (GUI) is provided for user input. However, the age-prediction program can also run without the graphical interface at the command line under the Linux[®] or DOS[®] operating systems if batch processing of multiple thermal histories from other, more sophisticated, thermal models is desired. The source code for these programs is available on request and written using C++ and Qt.

TERRA – 1D and 2D thermal history calculations

The TERRA thermal calculation module is well suited for users to explore different erosion/exhumation scenarios and their influence on subsurface temperatures. The influence of different rates and durations of erosion, as well as topographic geometries, can be easily evaluated so users develop an intuition for crustal thermal processes.

Figure 1 illustrates the user interface, or menu, for the calculation of 1D transient thermal fields during erosion. This program can be used to predict sample cooling histories for different user defined rates and durations of erosion. It is particularly useful for evaluating the transient evolution of subsurface temperatures and cooling histories during the early stages (e.g., first 5 m.y.) of mountain building and erosion. The program operates by solving the 1D transient advection-diffusion equation for a homogeneous medium with no heat production (for details,

File Edit

1D Transient Erosion | 2D Periodic Topography Model

Boundary Conditions

Surface Temperature Celsius

Basal Temperature Gradient C/m

Model Geometry

Maximum Model Depth m

Thermal Properties

Diffusivity m²/s

Erosion

Rate mm/yr

Thermochronometer Age Output Options

Write files for TERRA Age Prediction

Thermal Output Options

Plot temperature history of rock exposed at surface at:
 Million yrs output time

Plot geotherms at output times of:

Million yrs - Time 1 (Youngest)

Million yrs - Time 2

Million yrs - Time 3

Million yrs - Time 4 (Oldest)

Plot the depth history of the isotherms:

Temperature 1 (C)

Temperature 2 (C)

Temperature 3 (C)

Temperature 4 (C)

Calculate Transient Solutions

Figure 1. TERRA interface for calculation of 1D transient thermal histories for variable erosion rates.

see Eqns. 6 and 7 in Ehlers 2005). Rock thermal histories are recorded as they approach the surface. User defined inputs include thermal boundary conditions and material properties, model geometry, and rate of erosion. Several plots are generated from this program, including: (1) the thermal history of exhumed samples (Fig. 2), (2) geotherms at different time intervals (Fig. 2), and (3) the depth history of user defined temperatures (e.g., closure temperatures). The cooling history of a rock exposed at the surface is written to an output file for loading into the age prediction program.

Figure 3 illustrates the TERRA user interface for calculating the steady-state 2D thermal field beneath periodic topography. This program can be used to determine the position of isotherms and rock cooling histories under uniformly eroding topography. This program is particularly useful for evaluating the curvature of closure isotherms beneath topography of different wavelengths and amplitudes and potential topographic effects on cooling ages. The program operates by solving the steady-state 2D advection-diffusion equation for a uniformly eroding medium with depth dependent radiogenic heat production and periodic topography (Manktelow and Grasemann 1997). User defined inputs include thermal boundary conditions,

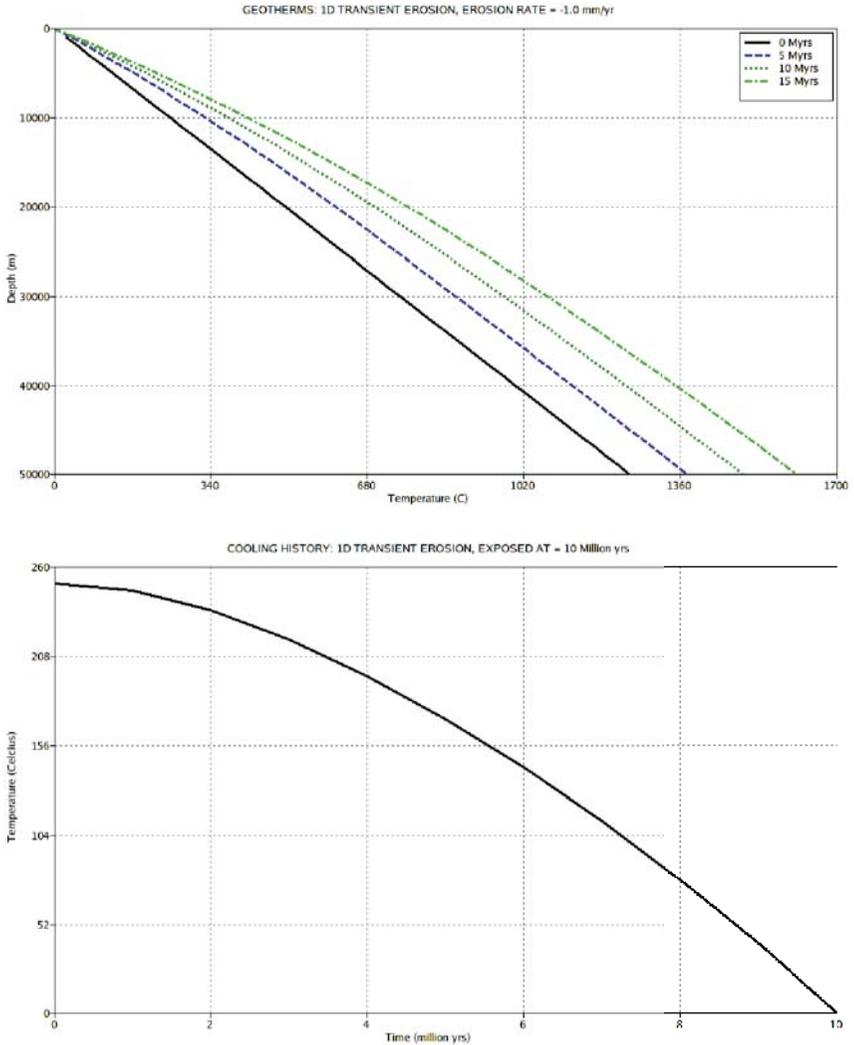


Figure 2. Example of TERRA predicted geotherms (top) and exhumed sample thermal history (bottom) plots from the 1D transient thermal calculation.

model geometry (topographic wavelength and amplitude), erosion rate, and material properties. Two plots are generated from this program: (1) The steady-state cooling history of rocks exposed between a ridge and adjacent valley bottom, and (2) the topography and steady-state position of user defined isotherms beneath the topography. Thermal histories of samples exposed between a ridge and valley are output to a file for loading into the age prediction program (see below).

All plots generated in this 2D periodic topography and the 1D transient erosion menus have options to print or save the plot. Other options available in the plot windows include the ability to zoom in and out to different parts of the plot. The menus also include default input parameters to help users unfamiliar with common thermal properties of rocks use the programs.

File Edit

1D Transient Erosion | 2D Periodic Topography Model

Erosion

Erosion rate mm/yr

Thermal Output Options

Plot temperature histories of rocks exposed at surface

Plot Isotherms and Topography

Define Isotherms to output

Isotherm 1 (Celsius)

Isotherm 2 (Celsius)

Isotherm 3 (Celsius)

Isotherm 4 (Celsius)

Thermochronometer Age Output Options

Write files for TERRA Age Prediction

Boundary Conditions

Surface temperature Celsius

Lithosphere base temperature Celsius

Lithosphere base depth m

Surface temperature lapse rate Celsius/m

Model Geometry

Topography wavelength m

Horizontal width m

Topography amplitude m

Maximum depth of calculation m

Thermal Properties

Diffusivity m²/s

Density of crust kg/m³

Specific heat J/kg/K

Surface volumetric heat production W/m³

Heat production characteristic depth m

Calculate Steady State Solution

Figure 3. TERRA input window for calculating steady-state cooling histories beneath 2D periodic topography.

TERRA – thermochronometer age prediction

The TERRA program also calculates predicted low-temperature thermochronometer ages from user defined thermal histories. Predicted ages for several thermochronometer systems are possible including: apatite and zircon (U-Th)/He ages and ⁴He concentration profiles across grains, multi-kinetic apatite fission track ages, and zircon fission track ages. Zircon fission track ages are calculated using an effective closure temperature.

Figure 4 shows two example input ‘tabs’ for the TERRA age prediction module. The first step in using the age prediction module is to load in files with rock thermal and coordinate position (optional) histories. The thermal and coordinate history for either a single sample, or for multiple samples, can be loaded to calculate predicted ages. The ability of this program to load multiple thermal histories for batch processing predicted ages is particularly useful for interpreting cooling histories calculated from more complex 2D or 3D thermal models (e.g., Ehlers and Farley 2003, Ehlers et al. 2003). After a thermal history is loaded, any or all of the thermochronometer ages listed at the top of the window can be calculated.

The figure displays two screenshots of the TERRA software interface. The top screenshot shows the 'Input Parameters' window for loading thermal history input files. The window has a title bar 'TERRA - Input Parameters' and a menu bar 'File Edit'. Below the menu bar are five tabs: 'General Settings', 'Apatite (U-Th)/He Input', 'Zircon (U-Th)/He Input', 'Multi-directional Apatite Fission Track Input', and 'Zircon Fission Track Input'. The 'Apatite (U-Th)/He Input' tab is selected. The main area contains several input fields with '...' buttons: 'Input File(s) (Generic Model)', 'Coordinate History of Vertices', 'Coordinate History of Vertices', 'Coordinate History of Vertices', 'Final Age & Coordinates', 'Final Ages (All Samples)', and 'Final File Coordinates (All Samples)'. On the right side, there is a 'Global Variable Settings' section with 'Additional Time to Add to Thermal History (My)' set to '0.0' and 'Time Step Size (years)' set to '100000'. At the bottom, there are three buttons: 'Minimum Apatite (U-Th)/He Input', 'Calculate Selected Ages', 'Calculate All Ages', and 'Exit'.

The bottom screenshot shows the 'Apatite (U-Th)/He Input' window for age prediction. The window has the same title bar and menu bar. The 'Apatite (U-Th)/He Input' tab is selected. The main area contains several input fields: 'Initial Diffusivity (D_0) (cm^2/yr)' set to '10.000', 'Effective Diffusivity (D_eff) (cm^2/yr)' set to '55.0', 'Grain Radius (micrometers)' set to '12.50', '230Th Homogeneous Concentration (ppm)' set to '13', and '232Th Homogeneous Concentration (ppm)' set to '27'. There is a checkbox for 'Activate Variable 230Th, 232Th Concentration (ppm)' which is unchecked. At the bottom, there are three buttons: 'Calculate Age', 'Minimum Apatite (U-Th)/He Input', 'Calculate Selected Ages', 'Calculate All Ages', and 'Exit'.

Figure 4. TERRA input windows for loading thermal history input files (top) and apatite (U-Th)/He age prediction (bottom). The window tabs for other thermochronometer systems have similar layouts.

The methods used for calculating each of the thermochronometer ages are as follows:

- *Apatite and zircon (U-Th)/He ages:* (U-Th)/He ages are calculated by solving the transient spherical ingrowth diffusion equation for homogeneous distributions of U and Th, and temperature dependent diffusivity (e.g., Farley 2000; Reiners et al. 2004). The equation is solved using a spherical finite element model as described in Ehlers et al. (2001, 2003).
- *Apatite fission track ages:* Apatite fission track ages are calculated using the mutikinetic annealing model of Ketchum et al. (1999, 2000). This model is similar to

the HeFTy program discussed later and accounts for variable annealing behavior as it correlates to etch pit width (D_{par}). Apatite fission track ages are calculated following the approach developed by Fuller (2003).

- *Zircon fission track ages*: Unlike apatite, a well developed annealing model for zircon fission tracks does not exist. As a consequence, TERRA calculates zircon fission track ages using an effective closure temperature (Dodson 1973, 1979; see also Brandon and Vance 1992; Brandon et al. 1998; and Batt et al. 2001). Zircon fission track ages are also calculated following the approach developed by Fuller (2003).

Calculated ages and coordinates of each sample (if provided in the input files) are written as output. Users can define their own kinetic parameters for (U-Th)/He and fission track age prediction, or use the default values to get started quickly.

HEFTY: FORWARD AND INVERSE MODELING THERMOCHRONOMETER SYSTEMS

Contributor: R. Ketcham (ketcham@mail.utexas.edu)

HeFTy is a computer program for forward and inverse modeling of low-temperature thermochronometric systems, including apatite fission-track, (U-Th)/He, and vitrinite reflectance. Fission-track and (U-Th)/He calculations are described in Ketcham (2005), and vitrinite reflectance is calculated using the EasyRo% method of Sweeney and Burnham (1990). HeFTy can simultaneously calculate solutions for up to seven thermochronometers. In addition to data analysis, HeFTy can also be an instructional aid, as it allows easy, interactive comparisons among thermochronometric systems and their parameters. It reproduces and extends the functionality of AFTSolve (Ketcham et al. 2000), and is intended to fully replace that program. It runs on the Windows® operating system. Figure 5 shows an example screen from HeFTy, with one file window open. Each file window in HeFTy corresponds to a single sample or locality, which can have associated with it multiple thermochronometers. To create a model, use one of the 3 “new” buttons on the top left of the task bar: the first creates a “blank” model (no thermochronometers), the second creates an AFT model, and the third a (U-Th)/He model. Additional thermochronometers can be included by clicking on the “+” button and selecting the type desired. Up to seven thermochronometers can be added.

For each thermochronometer, a new tab page is created, allowing model parameters to be changed and data to be entered for fitting. Whenever a model is added, this tab page is automatically brought to the front. To generate numbers, go to the “Time-Temperature History” tab. Clicking and dragging in the time-temperature history graph causes the forward model to run for all thermochronometers.

Data to be compared to forward modeling results or fitted using inversion can be typed directly into the program interface, and tabular data (such as fission-track lengths and single-grain ages) can be transferred from a table or spreadsheet using the clipboard (i.e., cutting and pasting). The easiest and most foolproof way to enter such data is using tab-delimited text files, which can be exported from any spreadsheet program. Included with the HeFTy distribution is the Microsoft Excel® file “Import templates.XLS”, which contains examples of all of the various input formats HeFTy supports.

The inverse modeling module is accessed by clicking the button to the right of the “+” button. A new window comes up for controlling the inversion processing (Fig. 6), and mouse clicks and motions in the time-temperature history graph create box constraints through which inverse thermal histories are forced to pass. Constraints can overlap, although rules are enforced to ensure that they occur in an unambiguous sequence. The amount of complexity

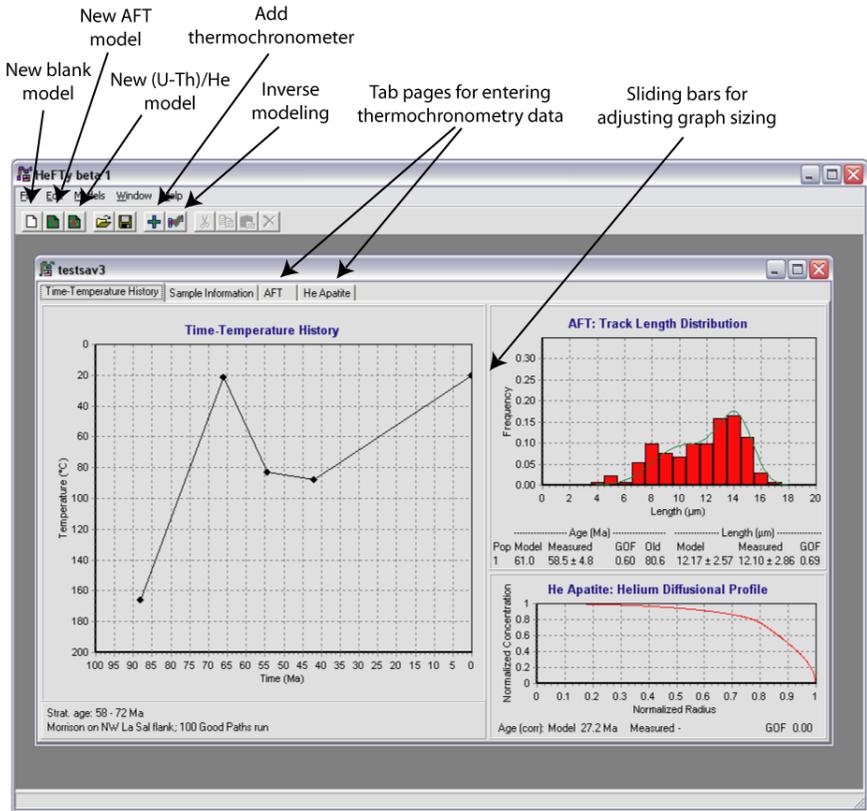


Figure 5. The HeFTy user interface.

allowed between each constraint (see Ketcham 2005) is controllable by right-clicking on the label in the middle of the line segments connecting constraint midpoints. In the example shown here, the first (leftmost) code of “1P” indicates that the time-temperature path segment is halved one time, with “intermediate” complexity; “2G/5” indicates that the segment is halved twice (into four sub segments), with the randomizer favoring a “gradual” history with a maximum heating rate of 5 °C/m.y.; and “3E/10” indicates that the segment is halved three times with the possibility for “episodic” histories (prone to sudden changes), but with a maximum cooling rate at all times of 10 °C/m.y.

FTINDEX: INDEX TEMPERATURES FROM FISSION TRACK DATA

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FTIndex is a program for calculating index temperatures and lengths that describe the geological time scale predictions of fission-track annealing models, as proposed by Ketcham et al. (1999). It is written in the C programming language. Both an executable version (for Windows®) and the source code are available for download.

Three index temperatures describe high-temperature annealing behavior. The fading temperature (T_F) is the downhole temperature required to fully anneal a fission-track population

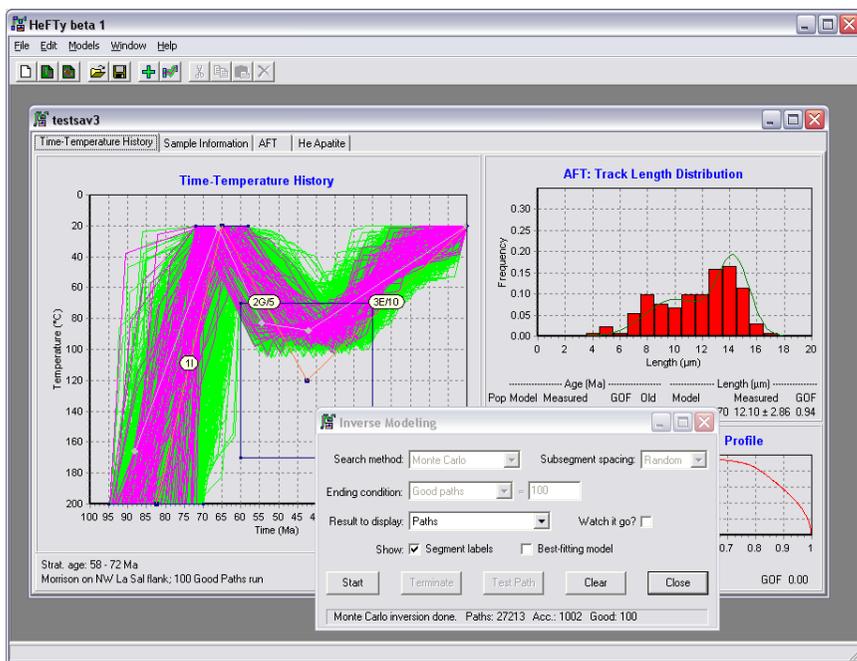


Figure 6. HeFTy inverse modeling mode.

after a certain number of millions of years, signified by the second subscript. For example, $T_{F,30}$ indicates the temperature required to fully anneal a population of fission tracks after 30 million years. The closure temperature (T_C) is the temperature experienced by a mineral at the time given by its age, assuming a constant-rate cooling history given by the second subscript—for example, $T_{C,10}$ means closure temperature given a 10 °C/m.y. cooling history. The total annealing temperature, T_A , is the temperature at which a fission-track population, fully anneals given a constant heating rate; it is equivalent to the oldest remaining population after a constant cooling episode. Again, the second subscript gives the heating/cooling rate. For both T_C and T_A , cooling is assumed to stop at 20 °C.

Low-temperature annealing behavior is modeled by estimating fission-track length reduction given a proposed time-temperature history. The best-constrained low-temperature history is from Vrolijk et al. (1992), which used apatites from deep-sea drill cores from the East Mariana Basin and utilized proposed time-temperature histories based on independent evidence. Two histories are provided by Vrolijk et al. (1992), which are end-members the bound uncertainties in rifting time in the East Mariana Basin. FTIndex calculates reduced length for both end-member cases and the average between them. To convert these to actual lengths, they must be multiplied by an estimated initial track length. The mean length of apatites measured by Vrolijk et al. (1992) was $14.6 \pm 0.1 \mu\text{m}$. Note that if an annealing model is based on *c*-axis projected lengths then the results will have to be converted to unprojected means to be compared to this value; this can be done with the relation:

$$r_m = 1.396r_c - 0.4017 \quad (1)$$

In general, to match the Vrolijk et al. (1992) data to within the uncertainty of the initial track length, the reduced length value for non-projected lengths should be in the range 0.89–

0.92, and reduced c -axis projected lengths should be in the range 0.92–0.95. A second low-temperature test is for Fish Canyon tuff, for which the assumed thermal history is a constant 20 °C for 27.8 million years.

FTIndex program operation

The program works by reading a text file that contains the coefficients describing one or more annealing model. It then calculates the index temperatures and writes them to a tab-delimited text file called bench.txt.

An example input file called IndexTest.txt has been provided in Table 2 to illustrate the file format. The basic format is a tab-delimited text file, with eleven columns and the first line a series of headers as shown above. The first column is a model name that will be repeated in the output file. The name should have no spaces. The second column is a numerical code signifying the form of the modeling equation; this form defines the meaning of the numbers in columns six through eleven, marked c_0 through c_5 . The third column denotes whether the model describes mean length or mean c -axis projected length; if the former it should be zero, otherwise one. The fourth and fifth columns are for r_{mr0} and κ parameters to translate lengths from one form of apatite to another (Ketcham et al. 1999), according to the equation:

$$r_{lr} = \left(\frac{r_{mr} - r_{mr0}}{1 - r_{mr0}} \right)^\kappa \quad (2)$$

where r_{lr} is the reduced length of a less-resistant apatite, and r_{mr} is the reduced length of the more-resistant apatite whose annealing is described by parameters c_0 through c_5 . If a conversion such as this is not desired then set r_{mr0} to 0 and κ to 1.

Unless otherwise noted, for all model equations, time (t) is in seconds and temperature (T) is in Kelvin, and r denotes reduced length while l denotes mean length. The model codes and forms are:

0: Fanning linear, based on Laslett et al. (1987) and Crowley et al. (1991).

$$\frac{\left[\frac{(1 - r^{c_5})}{c_5} \right]^{c_4} - 1}{c_4} = c_0 + c_1 \frac{\ln(t) - c_2}{(1/T) - c_3} \quad (3)$$

1: Fanning curvilinear, based on Crowley et al. (1991) and Ketcham et al. (1999).

$$\frac{\left[\frac{(1 - r^{c_5})}{c_5} \right]^{c_4} - 1}{c_4} = c_0 + c_1 \frac{\ln(t) - c_2}{\ln(1/T) - c_3} \quad (4)$$

Table 2: Example FTIndex input file format.

Name	Model	Lc	rmr0	kappa	C0	C1	C2	C3	C4	C5
L87Dur	0	0	0	1	-4.87	0.000168	-28.12	0	0.35	2.7
C90Dur	2	0	0	1	1.81	0.206	40.6	16.21		
LG96Fap	3	0	0	1	16.713	-4.879	0.000187	-33.385	0.000295	0.3333
K99DRLm	1	0	0	1	-106.18	2.1965	-155.9	-9.7864	-0.48078	-6.3626
K99RNLc	1	1	0	1	-61.311	1.292	-100.53	-8.7225	-0.35878	-2.9633
K99MLcRN	1	1	0.846	0.179	-19.844	0.38951	-51.253	-7.6423	-0.12327	-11.988
K99MLc165	1	1	0.84	0.16	-19.844	0.38951	-51.253	-7.6423	-0.12327	-11.988

2: Model of Carlson (1990).

$$l_{as} = c_3 - c_0 \left(\frac{kT}{h} \right)^{c_1} \exp \left(\frac{-c_1 c_2}{RT} \right) t^{c_1} \quad (5)$$

Where l_{as} is mean length due to axial shortening, k is Boltzmann's constant (3.2997×10^{-27} kcal·K⁻¹), h is Planck's constant (1.5836×10^{-37} kcal·s), and R is the universal gas constant (1.987×10^{-3} kcal·mol⁻¹·K⁻¹). Note that there are only four fitted parameters in this model, and thus only four should be entered in the file; columns 10 and 11 should be left blank.

3: Model of Laslett and Galbraith (1996).

$$l = c_0 \left[1 - \exp \left(c_1 + c_2 \frac{\ln(t) - c_3}{(1/T) - c_4} \right) \right]^{c_5} \quad (6)$$

Following their convention, in this case the time units are hours rather than seconds. If one fits the model using seconds, as with the other equations listed here, simply add $\ln(3600) = 8.18869$ to c_3 .

BINOMFIT: A WINDOWS® PROGRAM FOR ESTIMATING FISSION-TRACK AGES FOR CONCORDANT AND MIXED GRAIN AGE DISTRIBUTIONS

Contributor: Mark T. Brandon (mark.brandon@yale.edu)

The BINOMFIT program calculates ages and uncertainties for both concordant and mixed distributions of fission-track (FT) grain ages. The current program runs on the Windows® platforms. It incorporates features from two older DOS programs, called ZETAAGE and BINOMFIT. The ZETAAGE algorithm provides an exact estimation of FT ages and uncertainties (Sneyd 1984), regardless of track density. This capability is essential for estimating ages for samples with low track densities, which is common in young FT apatite samples (< ~15 Ma). The BINOMFIT algorithm is based on the decomposition method of Galbraith and Green (1990). An automated search routine has been added to the Windows® version of BINOMFIT, which automatically determines the optimal number of components in a FT grain-age distribution. This feature makes the program much easier to use for beginners. The original DOS versions of BINOMFIT and ZETAAGE are still maintained given that they are sometimes faster to use for experts. The source code for these programs is available on request.

Introduction to BINOMFIT

A common problem in FT dating is the interpretation of discordant fission-track grain age (FTGA) distributions. Discordance refers to the situation where the variance of the grain ages in FTGA distribution is greater than expected for analytical error alone. The widely used χ^2 test provides the main method for assessing if a distribution is "over-dispersed" relative to the expectation for count statistics for radioactive decay (Galbraith 1981).

Mixed distributions are expected for samples that have "detrital" FT ages, such as a sandstone with unreset zircon FT ages. Discordance is sometimes observed in zircon FT dating of volcanic tuffs, where the cause is likely due to contamination by older zircons.

Reset FT samples are also commonly discordant. In some cases, the discordance is taken as evidence for partial resetting, but the cause is more commonly due to differences in annealing properties, as caused by variations in composition for apatite or variations in

radiation damage for zircon. Heterogeneous annealing is expected for reset sandstones given that the dated apatites and zircons are derived from a variety of sources (Brandon et al. 1998), but this result is also found in some plutonic rocks as well, where one might expect that the dated mineral would be more homogeneous (O'Sullivan and Parrish 1995).

The binomial "peak-fitting" method of Galbraith and Green (1990) and Galbraith and Laslett (1993) is an excellent method for decomposing a mixed FT grain age distribution. This method was implemented by Brandon (1992) in a DOS program called BINOMFIT. The binomial peak-fitting method has been extensively used over the last 15 years and works very well for real FTGA distributions. A big advantage of the method is that it provides a one-component solution that is equivalent to the FT pooled age. Thus, the program works equally well for concordant and mixed FTGA samples.

Galbraith and Laslett (1993) introduced the term "minimum age," which can be loosely viewed as the pooled age of the largest concordant fraction of young grain ages in a FTGA distribution. Binomial peak fitting can also be used to estimate the minimum age of a distribution—equal to the youngest component in the distribution—while at the same time providing information about older components.

The FT minimum ages have been found useful for a variety of studies. For detrital zircon FT studies of volcanoclastic rocks, the minimum age is commonly a useful proxy for the depositional age of the rock (Brandon and Vance 1992; Garver et al. 1999, 2000; Stewart and Brandon 2004). Likewise, the minimum age for a tuff can remove biases due to older contaminant grains. For reset rocks, the minimum age represents the time of closure for that fraction of grains with the lowest retention for fission tracks, such as fluorapatites in apatite FT dating (e.g., Brandon et al. 1998) and radiation-damaged zircons in zircon FT dating (e.g., Brandon and Vance 1992).

Using BINOMFIT

BINOMFIT is distributed in a compressed zip file, called BinomfitInstall.zip. You need to download the file to your system, and place it in a temporary directory. Close all non-essential programs in Windows® to avoid conflicts with active processes during the setup. Double click the file to launch the decompression process, which will create three files needed for the installation process: setup.exe, setup.lst, and binomfit.cab.

The setup process is launched by double clicking setup.exe. This will install BINOMFIT into your program files area (e.g., C:/Program Files/Binomfit), and will also create a group entry labeled BINOMFIT in the Start Menu. Within this group are short cuts to the BINOMFIT program, a ReadMe file (i.e., this document in html format), and Documentation (in Adobe pdf format). The remaining support files (Mscomctl.ocx, Comdlg32.ocx, Msvcr7.dll, Scrrun.dll, Msstdfmt.dll, Msdbrpr.dll) will be placed in the application subdirectory as well, to avoid conflict with system DLLs and OCXs. After the installation is complete, you can delete the setup files. The installation is registered in Control Panel. As a result, you can use the "Add and Remove Program" option in Control Panel to uninstall the entire package.

The distribution package contains detailed instructions about how to construct a data file for input. Also included are several different types of data files and examples of typical output.

Figure 7 shows the program after completion of an automatic search for an optimal number of best-fit peaks. The buttons on the menu bar can be used to select between different types of plots, including a density plot (as shown) or a radial plot.

The Print option in the File menu will send a full report of grain ages, best-fit solution and graphical copies of all plots to a designated printer. The printed output for the Mount Tom FT sample is shown in Figure 7 is included in the documentation.

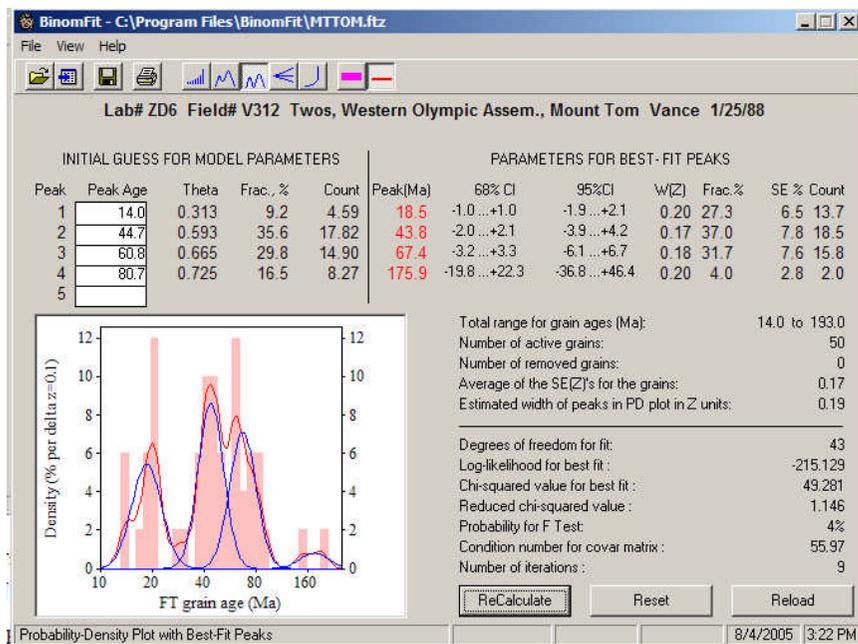


Figure 7. BINOMFIT best-fit solution for the Mount Tom zircon FT sample using the automatic peak-search mode.

The Save option in the File menu allows the user to save plot files, which can be imported into a graphics program (e.g., Excel®, SigmaPlot®) to prepare formal plots for publication. Plot files are available for probability density plots, radial plots, and $P(F)$ plots. The files are annotated to add in the construction of the relevant plot. Data file can be saved. This allows a permanent record of datasets that have constructed in BINOMFIT by removal of grain ages or by merging multiple data files.

PROGRAMS FOR ILLUSTRATING CLOSURE, PARTIAL RETENTION, AND THE RESPONSE OF COOLING AGES TO EROSION: CLOSURE, AGE2EDOT, AND RESPTIME

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CLOSURE, AGE2EDOT, and RESPTIME are a set of simple programs that were first developed in Brandon et al. (1998). They were designed to help demonstrate the influence of steady and transient erosion on fission-track (FT) cooling ages. The programs have since been extended to include (U-Th)/He and $^{40}\text{Ar}/^{39}\text{Ar}$ ages, as well as FT ages. The programs now include modern diffusion data for all of the minerals commonly dated for thermochronometry, ranging from He dating of apatite to Ar dating of hornblende.

CLOSURE is a standard Windows®-style program, whereas AGE2EDOT and RESPTIME are console-style programs. All of the programs are compiled for the Windows® operating system. Each consists of a single exe file. Setup involves copying the file into a suitable directory. The programs are started by double-clicking the file name. The programs require no input files. Rather, the user is guided by a set of prompts and questions to supply the necessary

input parameters for the calculation of interest. Results are output to a window for CLOSURE and to an output file for AGE2EDOT and RESPTIME. In all cases, the output is organized with tab-separated columns, so that it can be easily imported into a plotting program, such as Excel[®] or SigmaPlot[®].

The source code for the programs is available on request.

Methods for CLOSURE

The CLOSURE program provides a compilation of the data needed to calculate effective closure temperatures and partial retention temperatures for all of the minerals commonly dated by the He, FT, and Ar methods (Figure 8). Laboratory diffusion experiments have demonstrated that, on laboratory time scales, the diffusivity of He and Ar are well fit by the following relationship:

$$D = D_0 \exp \left[\frac{-E_a - PV_a}{RT} \right] \quad (7)$$

where D_0 is the frequency factor ($\text{m}^2 \text{s}^{-1}$), E_a is the activation energy (J mol^{-1}), P is pressure (Pa), V_a is the activation volume ($\text{m}^3 \text{mol}^{-1}$), T is temperature (K), R is the gas law constant ($8.3145 \text{ J mol}^{-1} \text{ K}^{-1}$), and D is the diffusivity ($\text{m}^2 \text{s}^{-1}$). The PV_a term is commonly set to zero, since its contribution is generally small relative to E_a . D_0 and E_a are compiled in Tables 1 and 2 for the main minerals dated by the He and Ar method.

The *partial retention zone* is defined in two ways. This concept was first introduced to account for partial annealing of fission tracks when held at a steady temperature. Laboratory heating experiments were used to define the time-temperature conditions that caused 90% and 10% retention of the initial density of fossil tracks. The retention behavior was considered for loss only, without regard for the production of new tracks during the heating event. We use the term loss-only PRZ to refer to this kind of partial retention zone for He, FT, and Ar dating. Figures 9, 10, and 11 show examples of loss-only PRZs. They help to illustrate the time and

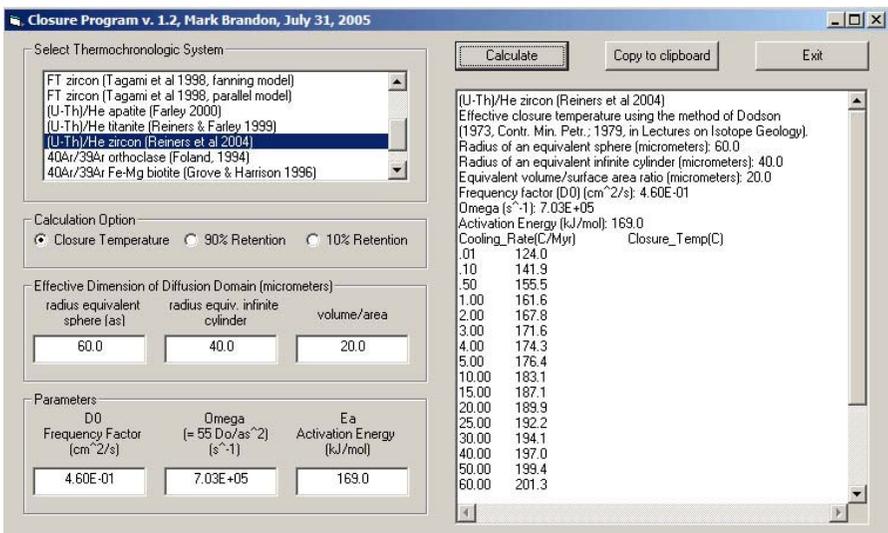


Figure 8. Screen image of the CLOSURE program showing a typical run result.

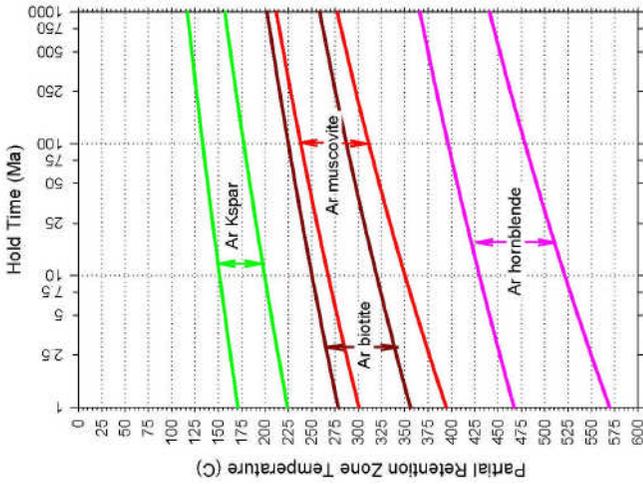


Figure 9. Loss-only PRZ for He dating methods calculated using CLOSURE.

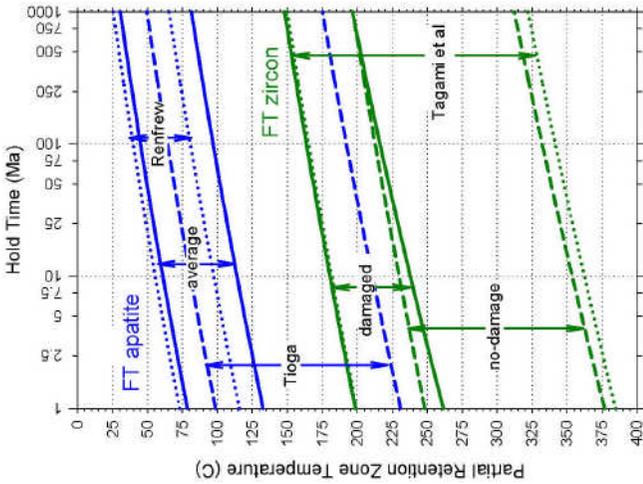


Figure 10. Loss-only PRZ for FT dating calculated using CLOSURE.

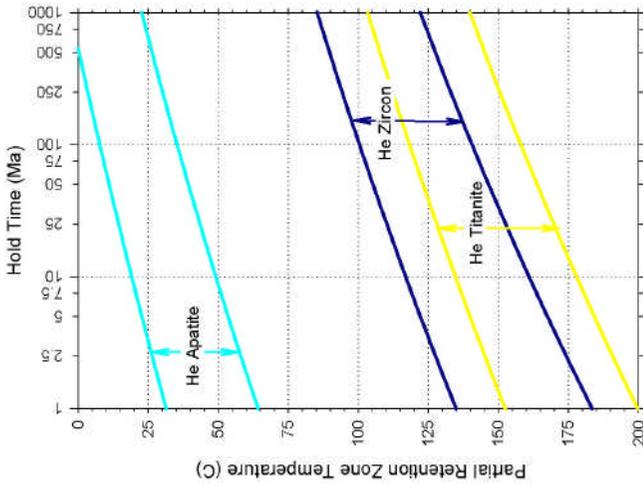


Figure 11. Loss-only PRZ for Ar dating calculated using CLOSURE.

temperature conditions needed to fully preserve or fully reset a He, FT, or Ar cooling age. The loss-only PRZ is calculated for He and Ar dating using the exact version of the loss-only diffusion equation (spherical geometry) from McDougall and Harrison (1999). The equations require D_0 and E_a as parameters, as given in Tables 3 and 4.

Wolf and Farley (1998) defined a different kind of PRZ, one that accounted for both production and loss of the ^4He , FT, or ^{40}Ar . The limits of the loss-and-production PRZ are defined by the temperatures needed to maintain a He, FT, or Ar age that is 90% or 10% of the hold time. The time-temperature conditions associated with this 90% and 10% retention are determined using the spherical He loss-and-production equation. The equations require D_0 and E_a as parameters. This kind of PRZ is useful for considering how the measured age for a thermochronometer will change down a borehole, as a function of downward increasing but otherwise steady temperatures.

Table 3. Closure parameters for He and FT dating.

<i>Method (references)</i>	E_a (kJ mol^{-1})	D_0 ($\text{cm}^2 \text{s}^{-1}$)	a_s^4 (μm)	Ω^5 (s^{-1})	$T_{c,10}^6$ ($^{\circ}\text{C}$)
(U-Th)/He apatite (Farley 2000)	138	50	60	7.64×10^7	67
(U-Th)/He zircon (Reiners et al. 2004)	169	0.46	60	7.03×10^5	183
(U-Th)/He titanite (Reiners and Farley 1999)	187	60	150	1.47×10^7	200
FT apatite ¹ (average composition ²) (Ketcham et al. 1999)	147	—	—	2.05×10^6	116
FT Renfrew apatite ³ (low retentivity) (Ketcham et al. 1999)	138	—	—	5.08×10^5	104
FT Tioga apatite ³ (high retentivity) (Ketcham et al. 1999)	187	—	—	1.57×10^8	177
FT apatite (Durango) (Laslett et al. 1987; Green 1988)	187	—	—	9.83×10^{11}	113
FT zircon ¹ (natural, radiation damaged) (Brandon et al. 1998)	208	—	—	1.00×10^8	232
FT zircon (no radiation damaged) (Rahn et al. 2004; fanning model)	321	—	—	5.66×10^{13}	342
FT zircon (Tagami et al. 1998; fanning model)	324	—	—	1.64×10^{14}	338
FT zircon (Tagami et al. 1998; parallel model)	297	—	—	2.56×10^{12}	326

Footnotes:

1) Recommended values for most geologic applications.

2) Average composition was taken from Table 4 in Carlson et al. (1999). Equation 6 in Carlson et al. (1999) was used to estimate $r_{mro} = 0.810$ for this composition. Closure parameters were then estimated using the HeFTy program (Ketcham 2005).

3) Closure parameters were estimated from HeFTy and $r_{mro} = 0.8464$ and 0.1398 for Renfrew and Tioga apatites, respectively, as reported in Ketcham et al. (1999).

4) a_s is the effective spherical radius for the diffusion domain. Shown here are typical values.

5) Ω is measured directly for FT thermochronometers, and is equal to $55D_0a_s^{-2}$ for He and Ar thermochronometers.

6) $T_{c,10}$ is the effective closure temperature for 10°C/m.y. cooling rate and specified a_s value.

Table 4. Closure parameters for Ar dating.

<i>Method</i> (<i>references</i>)	E_a (kJ mol^{-1})	D_0 ($\text{cm}^2 \text{s}^{-1}$)	a_s^1 (μm)	Ω^2 (s^{-1})	$T_{c,10}^3$ ($^{\circ}\text{C}$)
$^{40}\text{Ar}/^{39}\text{Ar}$ K-feldspar (orthoclase) (Foland 1994)	183	9.80×10^{-3}	10	5.39×10^5	223
$^{40}\text{Ar}/^{39}\text{Ar}$ Fe-Mg biotite (Grove and Harrison 1996)	197	7.50×10^{-2}	750 (500)	733	348
$^{40}\text{Ar}/^{39}\text{Ar}$ muscovite (Robbins 1972; Hames and Bowring 1994)	180	4.00×10^{-4}	750 (500)	3.91	380
$^{40}\text{Ar}/^{39}\text{Ar}$ hornblende (Harrison 1981)	268	6.00×10^{-2}	500	1320	553

Footnotes:

1) a_s is the effective spherical radius for the diffusion domain. Shown here are typical values. Muscovite and biotite have cylindrical diffusion domains, with typical cylindrical radii shown in parentheses. For these cases, a_s is approximated by multiplying the cylindrical radius by 1.5.

2) Ω is equal to $55D_0a_s^{-2}$ for Ar thermochronometers.

3) $T_{c,10}$ is the effective closure temperature for 10 °C/m.y. cooling rate and specified a_s value.

The CLOSURE program estimates both types of PRZ for He and Ar methods. It only calculates the loss-only PRZ for FT methods. Annealing models, such as HeFTy (Ketchum 2005) could be used to calculate a loss-and-production PRZ for the FT apatite system, but there is no such model yet for annealing and production for the FT zircon system. The 90% and 10% retention isopleths are determined from time-temperature results from laboratory stepwise-heating experiments. The isopleths commonly have an exponential form,

$$t = \Omega^{-1} \exp\left[-\frac{E_a}{RT}\right] \quad (8)$$

where E_a is the activation energy, Ω is the normalized frequency factor, R is the gas law constant, T is the steady temperature (K), and t is the hold time (s). This can be recast into the typical Arrhenius relation,

$$\ln[t] = -\ln[\Omega] - \frac{E_a}{RT} \quad (9)$$

This approach was used to determine E_a and Ω for 90% and 10% retention minerals dated by the fission track method (Table 5).

Dodson (1973, 1979) showed that for a steady rate of cooling, one could identify an *effective closure temperature* T_c , which corresponds to the temperature at the time indicated by the cooling age measured for the thermochronometer (Fig. 12). We emphasize that T_c is only defined for the case of steady cooling through the PRZ, but this assumption is reasonable for many eroding mountain belts, given the narrow temperature range for the PRZ and the slow response of the thermal field to external changes. In contrast, this assumption will likely fail for areas affected by local igneous intrusions, hydrothermal circulation, or depositional burial.

Dodson (1973, 1979) estimated T_c using

$$\dot{T}(T_c) = \frac{-\Omega RT_c^2}{E_a} \exp\left[-\frac{E_a}{RT_c}\right] \quad (10)$$

where $\dot{T}(T_c) = (\partial T/\partial t)_{T=T_c}$ ($\dot{T} < 0$ for cooling), R is the gas law constant, and the normalized

Table 5. Parameters for FT partial retention zones.

<i>Method (references)</i>	<i>Retention Level</i>	<i>E_a (kJ mol⁻¹)</i>	<i>Ω⁴ (s⁻¹)</i>
FT apatite ¹ (average composition ²) (Ketcham et al. 1999)	90%	127	2.67 × 10 ⁵
	10%	161	1.55 × 10 ⁷
FT Renfrew apatite ³ (low retentivity) (Ketcham et al. 1999)	90%	124	1.91 × 10 ⁵
	10%	150	4.39 × 10 ⁶
FT Tioga apatite ³ (high retentivity) (Ketcham et al. 1999)	90%	140	1.41 × 10 ⁶
	10%	232	3.38 × 10 ¹⁰
FT Durango apatite (Laslett et al. 1987; Green 1988)	90%	160	1.02 × 10 ¹²
	10%	195	2.07 × 10 ¹²
FT zircon ¹ (natural, radiation damaged) (Brandon et al. 1998)	90%	225	2.62 × 10 ¹¹
	10%	221	1.24 × 10 ⁸
FT zircon (no radiation damage) (Rahn et al. 2004; fanning model)	90%	272	5.66 × 10 ¹³
	10%	339	5.66 × 10 ¹³
FT zircon (Tagami et al. 1998; fanning model)	90%	231	1.09 × 10 ¹²
	10%	359	1.02 × 10 ¹⁵
FT zircon (Tagami et al. 1998; parallel model)	90%	297	5.94 × 10 ¹⁵
	10%	297	1.51 × 10 ¹¹

Footnotes:

1) Recommended values for most geologic applications.

2) Average composition was taken from Table 4 in Carlson et al. (1999). Equation 6 in Carlson et al. (1999) was used to estimate $r_{m0} = 0.810$ for this composition. PRZ parameters were then estimated using the HeFTy program (Ketcham 2005).

3) PRZ parameters were estimated from HeFTy and $r_{m0} = 0.8464$ and 0.1398 for Renfrew and Tioga apatites, respectively, as reported in Ketcham et al. (1999).

4) Ω is measured directly for FT thermochronometers

frequency factor Ω and activation energy E_a are closure parameters, as defined in Tables 3 and 4. The cooling rate at T_c is given by $\dot{T} = (\partial T / \partial z)_{T_c} \dot{\epsilon}(\tau_c)$, where $(\partial T / \partial z)_{T_c}$ is the thermal gradient at the closure isotherm, and $\dot{\epsilon}(\tau_c)$ is the erosion rate at τ_c , the time of closure.

For He and Ar dating, $\Omega = 55D_0/a_s$, where a_s is the equivalent spherical radius for the diffusion domain. Tables 3 and 4 list typical values for a_s , but the user will need to judge if a more suitable value is appropriate given the specifics about what has been dated. Most of the minerals dated by He and Ar have isotropic diffusion properties, meaning that He and Ar diffuse at equal rates in all directions (muscovite and biotite are exceptions that are discussed below). Furthermore, the diffusion domains are commonly at the scale of the full mineral grain. The dated minerals may have anisotropic shapes. As an example, zircons and apatites tend to occur as elongate prisms. We can calculate an approximate equivalent spherical radius using

$$a_s \approx 3 \frac{V}{A} \quad (11)$$

(Fechtig and Kalbitzer 1966; Meesters and Dunai 2002), where V and A refer to the volume and surface area of the mineral grain.

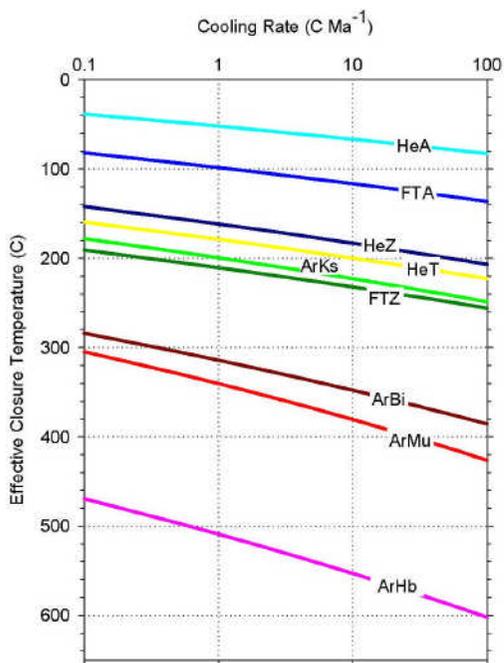


Figure 12. Effective closure temperatures calculated using CLOSURE.

Biotite and muscovite are anisotropic, with the fast direction of diffusion parallel to the basal plane, indicating cylindrical diffusion geometry. Equations are available to solve for cylindrical diffusion, but we have opted to approximate the solution by converting the cylindrical radius a_c of the mica grains into an equivalent spherical radius, where $a_s = 1.5 a_c$, and then using this radius with the spherical solution for the diffusion equations. These approximate scaling relationships are shown for the values under the label “Effective Dimensions of Diffusion Domain (micrometers).” These approximations are very good for calculating 90% retention and effective closure temperatures. They work less well for calculating the time-temperature conditions for 10% retention.

The Dodson equation can also be applied to the fission-track system (Dodson 1979). He recommended using E_a and Ω determined from the

50% retention isopleth from time-temperature heating experiments. Fission tracks contain a range of defects, created by the flight of the two energetic fragments created by the fission decay reaction of ^{238}U . This situation accounts for why the annealing process has a range of E_a values, which increase with increasing annealing of initial tracks. This observation is thought to mean that there is a range of activation energies needed to drive the diffusion involved in repairing this lattice damage (e.g., Ketchum et al. 1999). We do not know the size of the diffusion domain, which means that we cannot measure D_0 . Nonetheless, we can measure Ω , which is all that is needed to use the Dodson closure equation. Dodson (1979) argued that the 50% retention isopleth provides the best average values for E_a and Ω , given that the cooling path for closure requires moving through the PRZ.

We have estimated these parameters from a range of FT annealing experiments (Table 5). We have compared the T_c values calculated with the Dodson equation with those estimated by more complex FT models, such as HeFTy. In general, the Dodson estimates for T_c are within ~ 1 °C relative to those given by numerical models.

Methods for AGE2EDOT

AGE2EDOT estimates the cooling age for a thermochronometer that was exhumed by steady erosion at a constant rate (Fig. 13). The thermal field is represented by the steady-state solution for an infinite layer with a thickness L (km), a thermal diffusivity κ ($\text{km}^2 \text{Ma}^{-1}$), a uniform internal heat production H_T , a steady surface temperature T_s and an estimate of the near-surface thermal gradient for no erosion. These thermal parameters are usually estimated, at least in part, from heat flow studies. We use, as an example, thermal parameters for the active convergent orogen in the northern Apennines of Italy, where $L \sim 30$ km, $\kappa \sim 27.4 \text{ km}^2 \text{Ma}^{-1}$,

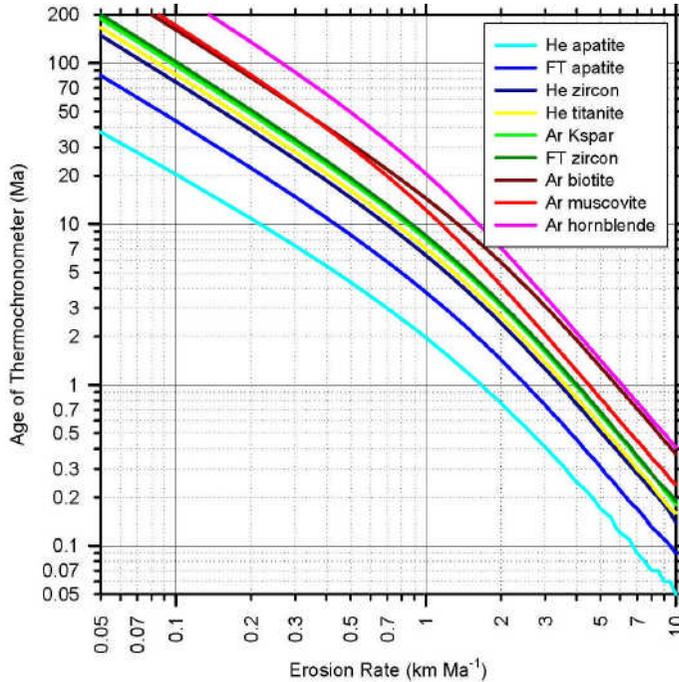


Figure 13. Age versus erosion rate for all of the major thermochronometers. Calculated using AGE2EDOT.

$H_T \sim 4.5 \text{ } ^\circ\text{C Ma}^{-1}$, $T_s \sim 14 \text{ } ^\circ\text{C}$, and the zero-erosion surface thermal gradient would be $\sim 20 \text{ } ^\circ\text{C km}^{-1}$. The calculated basal temperature is $540 \text{ } ^\circ\text{C}$, which is held constant throughout the calculation. Material moves through the layer at a constant velocity u . One can envision that this situation simulates a steady-state orogen where underplating is occurring at the same rate as erosion, with $u = \dot{\epsilon}$. The thickness of the orogen remains steady and the vertical velocity through the wedge would be approximately uniform and steady.

The thermal model provides a full description of the temperature and thermal gradient as a function of depth. The cooling rate is $\dot{T}(T_c) = (\partial T / \partial z)_{T_c} \dot{\epsilon}$. Given the cooling rate and the temperature with respect to depth, we can use the Dodson equation to solve for T_c , and for the depth of closure z_c . The predicted cooling age is given by $z_c / \dot{\epsilon}$.

AGE2EDOT gives a full prediction of how the cooling age for the specified thermochronometer will change as a function of erosion rate. Faster erosion causes isotherms, including the closure isotherm, to migrate closer to the surface. The steeper thermal gradient causes a faster rate of cooling and thus a greater T . The net effect is that the closure depth becomes shallower with faster erosion, but this effect is reduced by the response of the increase in T_c caused by faster cooling.

Brandon et al. (1998) provides more details about this calculation. Figure 13 is an example of the relationship between erosion rate and cooling ages for all of the major thermochronometers. The thermal parameters used are those discussed above for the northern Apennines. An example of the input data and results is given in the file: AGE2EDOT.output available online at the software download site associated with this chapter.

Methods for RESPTIME

RESPTIME calculates the migration of the closure isotherm due to an instantaneous change in erosion rate. The program is similar to AGE2EDOT but it uses a finite-difference algorithm to solve for the evolution of 1D thermal field in an infinite layer. Figure 14 shows plots of the response of all of the major thermochronometers to a instantaneous change from no erosion before 0 Ma to steady erosion at a rate of 1 km Ma⁻¹. Thermal parameters used are identical to the northern Apennines values used for the example for AGE2EDOT. The distribution package includes a sample output file from this example (see the file called RESPTIME.output). Note that L was increased to 50 km for the Ar muscovite and Ar hornblende calculations, in order to ensure that T_c remained within the layer for these high-temperature thermochronometers.

The motion of the closure isotherm is represented in Figure 14 by its normalized velocity, which is defined by the vertical velocity of the isotherm divided by the erosion rate. A normalized velocity of zero means that the closure isotherm has reached a steady-state position; whereas a normalized velocity of one means that the isotherm is moving upward at the same rate as the rock. There would be no cooling at this stage.

Figure 14 shows that the normalized velocity for the He thermochronometer slows down to <10% within 2.5 Ma following the start of fast erosion. In contrast, it takes 16 Ma for the Ar muscovite system to reach the 10% level. This example highlights the importance for using low-temperature thermochronometers for measuring erosion rates.

TASC: COOLING ONSET AGES AND EVENT TIMING IN NATURAL SAMPLES FROM FISSION TRACK LENGTH DATA

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Track age spectrum calculator (TASC) is an Microsoft Excel® worksheet built for Microsoft Windows® XP that provides a means of gaining additional information from the raw track length and apparent age data routinely collected for fission track samples. By recalculating the track density to incorporate the length-dependent probabilities, the user can determine the age of the oldest measured track—the “cooling onset” age—which is effectively the time the sample passed through the base of the partial annealing zone (PAZ) and began to retain tracks. Quantifying this age permits each individual track in the traditional length histogram to be allocated an equivalent age, thus allowing it to be recast as a “track age spectrum”. The calculations are independent of chemistry and mineralogy and the output incorporates uncertainties reflecting age error and anisotropy. While the time information is quantitative, the temperature information is largely qualitative. The “cooling onset age” and indicators of cooling style and timing extracted by this approach provide a very useful guide to the thermal history before inverse modeling of the sample is attempted. TASC enables robust histories to be rapidly developed, particularly in shield areas where stratigraphic and structural control may be minimal or absent. Other applications include: (1) rapid identification of timing in the simultaneous cooling of vertical profiles—the timing of which is frequently masked or ambiguous in those samples residing in or above the palaeo-PAZ; (2) use of the “cooling onset age” to contour maps of total exhumation (where suitably calibrated); (3) generation of “event” spectra (analogous to detrital zircon age spectra) from a regional series of samples. The method may also prove of significant value in the study of other minerals such as sphene and zircon, where annealing models are still evolving.

Background to the TASC program

The TASC approach is based on the logic of Laslett et al. (1982) who considered the probability of a track intersecting an arbitrary surface through a grain. They concluded that the

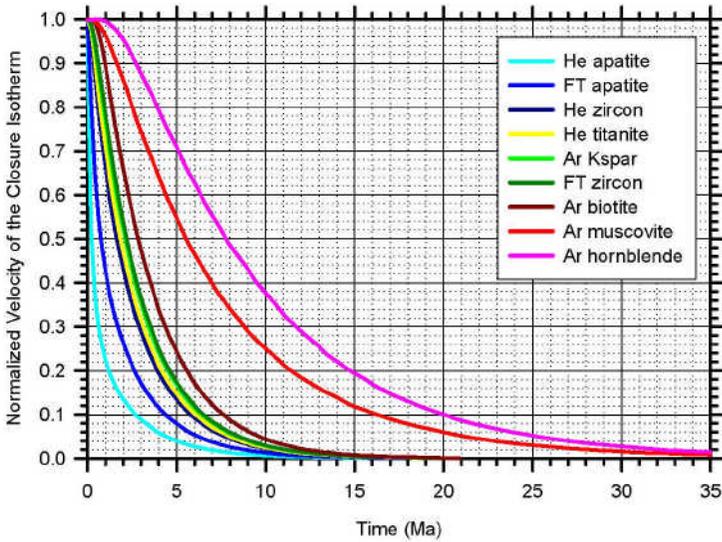


Figure 14. Response time of closure isotherms for the listed thermochronometers due to an instantaneous increase in erosion rate at time 0 Ma, from no erosion to 1 km Ma^{-1} . Calculated using RESPTIME.

sampling or intersection probability is directly proportional to the track length (i.e., a linear length-density relationship). Their argument was in essence, that a $16 \mu\text{m}$ track is twice as likely to intersect a polished surface, and thus be sampled in density measurements, as an $8 \mu\text{m}$ track and 4 times as likely to be sampled as a $4 \mu\text{m}$ track. Laslett et al. (1982) also provided a mathematically rigorous assessment of the treatment for the case of TINTS and TINCLES (Lal et al. 1969) routinely measured in samples.

If, for arguments sake, fission tracks in a given sample have an initial track length of $\sim 16 \mu\text{m}$, then the inverse of the Laslett et al. (1982) argument can be restated as follows: For a given “true” or debiased track-length distribution, the “true” number of $8 \mu\text{m}$ tracks that would have intersected the surface at formation length, will be double the observed amount, since because of annealing, there is only a 50% probability of measuring the shortened track. Similarly, to adjust for the observation probability of only 25%, the “true” number of $4 \mu\text{m}$ tracks will be four times the observed amount. This correction is equivalent to extending all tracks in a variable length distribution back to their initial formation length (Fig. 15). Once the true probability is determined for each measured length in the distribution (or each bin interval if only binned data are available), the recalculated total density of tracks that would be expected to intersect the surface is used to modify the traditional age equation (Fleischer et al. 1975).

Having determined the “cooling onset age”, it is a simple matter to rescale the traditional length histogram with the relationship between the number of track lengths and the total number of “rescaled tracks”. Each bin is allocated its appropriate number of rescaled tracks based on their intersection probability, which allows the boundary of each bin to be defined by a specific time. In order to allocate some measure of uncertainty (e.g., due to annealing anisotropy) to the result, the entire TASC procedure is repeated at one standard deviation (\pm) using the standard deviations recorded for Durango apatite by Green et al. (1986). This uncertainty gives a plausible, though not necessarily statistically robust, estimate of the uncertainty of the bin ages.

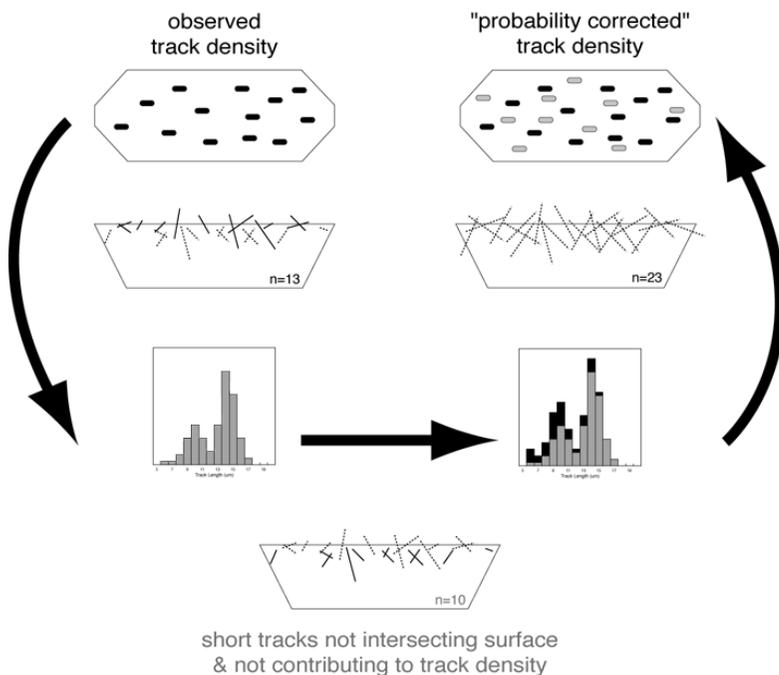


Figure 15. Schematic of the TASC calculation. Observed track density is a function of the intersection probability of the mixture of short and long tracks. When the density is adjusted for the expected intersections that would occur if all tracks retained their initial formation length, then the cooling onset age is revealed. This age reflects the point in time at which fission tracks began to be retained, rather than completely annealed, (nominally 110 °C) as the sample moved up through the crustal isotherms.

Applications of the TASC program

Recasting the traditional length histogram produces the “track age spectrum” which retains all the original thermal history information from the length histogram (Figs. 16 and 17) including, for example, the skewed distribution of an accelerated cooling or the bimodality of a reheating event (Gleadow et al. 1986). However, the track age spectrum also enables the timing of these events to be readily estimated, and in some cases gives an indication of the “severity” of a thermal perturbation.

When applied to vertical profiles, TASC analysis enables rapid identification of events recorded in samples both above and below a “break in slope.” Estimates of exhumation rates, particularly above a “break in slope”, can be derived from “onset cooling ages.” Semi-quantitative timing information extracted from the track age spectra of grouped samples (e.g., vertical profiles or localized tectonic blocks) can be effectively and concisely summarized on the event spectrum in much the same way as detrital zircon fission track age populations are illustrated in probability plots (Brandon 1992). This enables the user to readily identify important thermal events at one site and is a powerful means of evaluating the regional thermal histories. Because the TASC calculation is independent of chemistry and mineralogy, it has potential application in the study of other minerals such as zircon, where annealing models are still evolving.

By itself, the “cooling onset” age derived from TASC can be used as the basis of extended regional contour maps giving a large-scale overview of regional cooling histories. In contrast

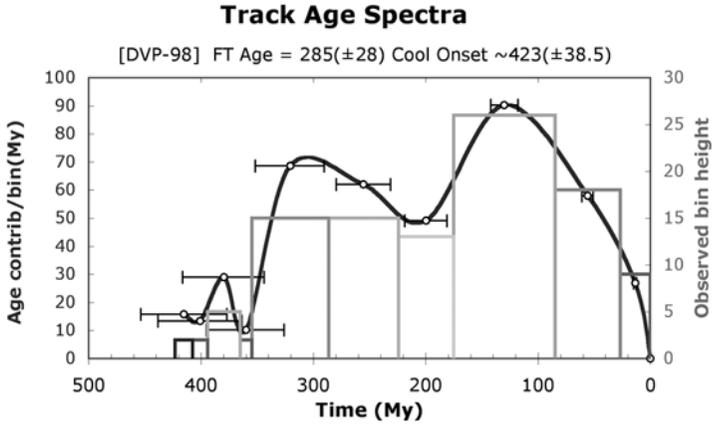


Figure 16. Track age spectrum for a cratonic sample with the complex thermal history (illustrated in Fig. 17). The spectrum retains the typical bimodal distribution seen in the traditional length histogram and indicative of a reheated sample. The TASC results are predict the style of cooling independently modeled using inverse methods (Fig. 17).

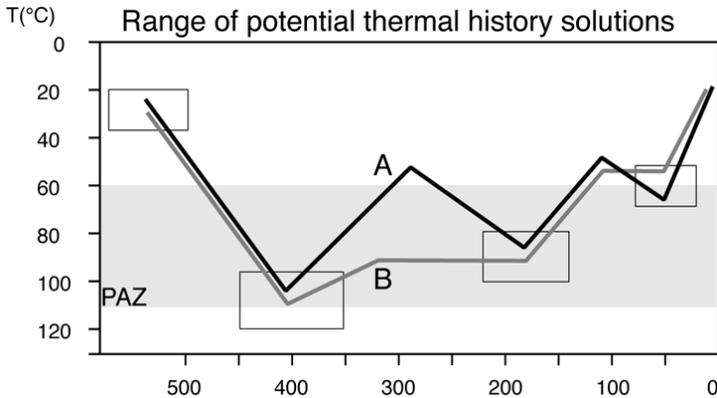


Figure 17. Range of thermal history solutions (curves A and B) for a sample from central Australia (Belton et al. 2004). The thermal histories were determined independently of the TASC solution (see Fig. 16) and are based on geological constraints and inverse modeling (MonteTrax; Gallagher 1995).

to traditional maps relying on apparent fission track ages, the cooling onset age provides an unambiguous indicator of the time that a sample either (1) entered the base of the PAZ or (2) began to retain tracks again following a thermal reset (e.g., Fig. 17). With some additional assumptions regarding composition and cooling rates, this information can be inverted to derive exhumation estimates for large areas.

The TASC approach should prove to be a powerful precursor to current well-established inverse modeling techniques such as MonteTrax (Gallagher 1995) and AFTSolve (Ketcham et al. 2000). It cannot replace these methods but will complement them, so that in many cases the additional information garnered from TASC will enable robust model histories to be rapidly developed.

Using the TASC program

The program is provided as an Microsoft Excel® worksheet to suit the Microsoft Windows® XP platform. No installation is required, simply copy the file to your hard drive, click on the file and it will open under Excel®. It is recommended that you create a permanent folder for the TASC file *before* you start it for the first time. This ensures that the macros in the work sheet remain correctly linked to the TASC toolbar and it provides a single location for the output text files as well. Users may have to alter security permissions on their computers to enable the Visual Basic® macros in this program to function.

TASC controls

TASC has its own tool bar and each of the control buttons is replicated in the worksheet. These controls permit the user to:

1. Clear previous input data prior to the next calculation.
2. Adjust spectrum x -axis. This may need to be done if the apparent fission track age input is altered during calculation.
3. Choose color plots for easy comparison between the length histogram and track age spectra or select black and white to print the plots directly from Excel®.
4. Export output as a text file (“sample name spectra”) containing the x and y ranges for plotting the spectra in other software packages.
5. Select from a choice of five quick examples showing the spectrum for different thermal history styles. These examples are based on both synthetic and real data. The user manual provides more detailed information on a number of complex examples with case histories.

TASC inputs

The following inputs are required for TASC to perform its calculation:

1. Binned lengths – these can be entered individually or pasted. Note, only lengths greater than 5 μm are used in the calculation...OR...
2. Individual track lengths – again these can be entered one at a time however most users will prefer to cut and paste. TASC will accept up to a maximum of 130 individual tracks.
3. Apparent fission track age in Ma
4. Error on the apparent age ($\pm 1 \sigma$) in Ma
5. Name of the sample.
6. Initial (or maximum) track length – closely approximating the formation length of fission tracks in the sample. The default is 16.3 μm , however in natural samples you may wish to use the longest individual length observed in the sample.

TASC outputs

Screen outputs from TASC are:

1. Cooling Onset Age – which marks the age of the oldest retained fission track.
2. Fission track density multiplier – which is used to adjust the traditional apparent fission track age.
3. Track age spectrum, consisting of age calibrated histogram bins (notice the bins now have differing widths) with an additional smoothed curve indicating the central value for each bin and error bars for each bin. This curve is useful for rapidly interpreting the results.

4. Traditional length histogram.
5. A text file is output on request and contains the input age, error and length bins as well as all the output data allowing for plotting in other packages.

DECOMP: FORWARD MODELING AGE EVOLUTION OF (U-TH)/HE AGES

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The program DECOMP is designed to calculate age evolution curves for U-Th-He thermochronology (Forward modeling). It is an amendment to the papers of Meesters and Dunai (2002a,b) and is described in Dunai (2005). DECOMP computes age evolution curves for spherical symmetry. It can also be used as an accurate approximation for other geometries if spheres of identical surface to volume ratio and properly transposed zonation of parent nuclides are used. Any results obtained with this program must be properly referenced if they are used in publications and presentations. Proper referencing is referring to *both* Meesters and Dunai (2002, part II) *and* the program (DECOMP; by A. Bikker, A.G.C.A. Meesters and T.J. Dunai).

The target audiences for DECOMP are beginners and experienced practitioners in thermochronology. The functionality of the software lends itself to several applications.

1. Qualitative assessment of how changes of sample parameters (diffusion parameters, surface/volume ratios, emission distance) and model temperature histories affect ages. This aspect is particularly useful for teaching/learning what the most sensitive parameters for a certain system are.
2. Quantitative forward modeling of any time temperature history.
3. Qualitative assessment of the effect of parent nuclide zonation.
4. Although DECOMP was originally designed for forward modeling of (U-Th)/He ages, forward modeling of any thermochronological system that is governed by volume diffusion, and of which the diffusion parameters (D_0 , E_a) of the radionuclide are known, is possible.

How to use DECOMP

DECOMP provides a user-friendly interface that allows repeated calculations of (U-Th)/He ages (e.g., Meesters and Dunai 2002). The results can be exported to standard spreadsheet programs. On first starting the program the user is asked to fill in, step by step, the parameters necessary for a computation. In most cases default values or exemplary temperature histories are supplied, which of course can be changed. Both the left and right buttons of the mouse can be used to have access to options (such as adding and/or editing points to the temperature histories). On finishing this introduction the actual window of DECOMP will appear. After the user quits DECOMP for the first time the introduction will not reappear on restarting DECOMP. Starting DECOMP is straightforward: double click on the icon of the executable file (DECOMP.EXE).

An example of the DECOMP program interface is shown in this volume (e.g., Fig. 3; Dunai 2005). There are several input options associated with this interface required for using the program:

1. Button panel
 - *Save* and *open* geometric parameters, temperature histories, constants and annotations.

- *Quit* the program.
 - *Recalculate* the age evolution diagram.
 - *Edit constants*: number of eigenvalues used for computation; activation energy (the non-SI unit [cal/mol] is used here as currently most values are still published in [cal/mol], for conversion 1 joule = 0.239 cal); pre-exponential factor D_0 [cm²/s].
2. Input parameters describing the geometry of a sample:
- *Sphere radius*: Radius (in microns) of a sphere of identical surface to volume ratio as the sample.
 - *Outer and inner zone radius*: Gives the outer and inner radius (in microns) of the zone containing the parent nuclides. The shape of the zone containing the parent nuclides is visualized by the red zone in the circle to the right of the input field that is changing simultaneously while changing values. Samples with a homogenous parent nuclide distribution have outer zone radius equal to the sphere radius and an inner radius of 0 microns.
 - *Emission distance*: Emission distance (in microns) of alpha particles.

Temperature history plot

The temperature and real time at the position of the tip of the cursor are indicated in the frame at the top right of the diagram. Note that the real time represents time elapsed since beginning of the model simulation. When using this plot, the following operations can be performed using the indicated mouse buttons:

- Right mouse button:
 - *copy* the numeric values of temperature history (comma-delimited table) to be pasted (e.g., in a spreadsheet program).
 - add and delete points to/from the temperature history
 - table edit: edit the numeric values of existing points of the temperature history
- Left mouse button:
 - drag axis to scale
 - drag existing points

Age evolution plot

Initially the age-evolution diagram is blank. After pressing the recalculation button the age evolution is calculated for the current temperature history. The numeric values curve can be copied (right mouse button) and pasted into a spreadsheet program (table comma delimited). The calculated age and real time at the position of the tip of the cursor are given in the frame at the top right of the diagram. Note, in this plot the calculated age represents the age as it would be calculated from U, Th and He concentrations in a sample.

4DTHERM: THERMAL AND EXHUMATION HISTORY OF INTRUSIONS

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4DTHERM v.1.2 is an inverse thermal modeling program. It uses a 2D explicit finite difference solution which addresses conduction cooling, latent heat of crystallization/fusion, convection within magma bodies, and hydrothermal circulation induced by magma intrusion as well as exhumation and erosion processes. 4DTHERM was implemented in Java

programming language and is platform-independent. It has been tested in Windows® ME, XP and Linux/Unix OS, and should run in Mac® OS X and other operating systems. It has a interactive graphical user interface (GUI) for constructing geologic units, inputting and modifying computational parameters, editing model scenarios, and controlling modeling procedures. It provides graphic windows (Fig. 18) to observe the cooling process in a 2D cross section and to view the plotted thermal histories of pre-defined positions. Final modeling results can be saved in formatted text files whereas step-by-step running status is displayed in the status board.

4DTHERM applications

The primary application of this model is to derive thermal and exhumation histories of igneous intrusions directly from multiple thermochronometers. 4DTHERM quantifies a number of parameters related to the dynamic processes of magmatic-hydrothermal cooling, timing and duration of hydrothermal activity, and denudation histories of igneous intrusions and related mineralization (McInnes et al. 2005a,b). It also computes both cooling and exhumation histories of igneous intrusions. A brief overview of the processes simulated is as follows:

Modeling of magmatic-hydrothermal cooling. 4DTHERM simulates the conductive and convective cooling processes of igneous bodies. It computes the distributions and variations of temperature in both igneous bodies and country rocks throughout the whole cooling process. It records the time and duration of magmatic-hydrothermal activities induced by intrusions.

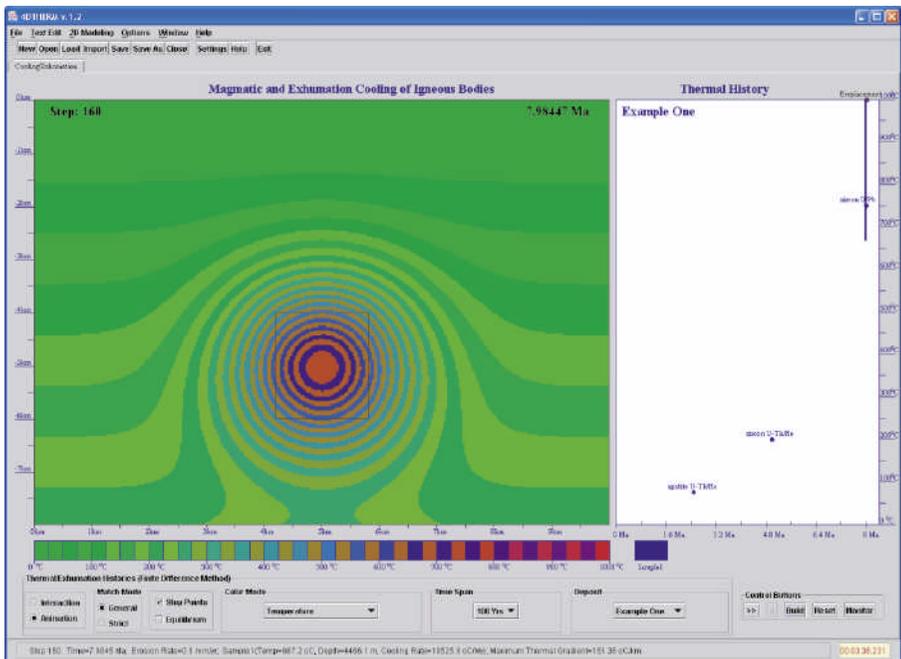


Figure 18. A screenshot of 4DTHERM v.1.2. The large window on the left displays the distribution of temperature in vertical cross section with an isotherm of 25 °C for each color band, and the black rectangle in the middle of the window indicates the position of a cooling igneous body. The white window on the right is plotting the cooling curve for a sample from the intrusion and the three small dots are the input age data obtained from sample of the intrusion or country rock used to constrain the cooling curve. Below the two windows are the temperature legend, control panel and status board, respectively.

It also records the cooling histories and calculates the cooling rates for some pre-defined positions (e.g., sample positions in igneous bodies and/or country rocks).

The algorithm behind the model solves a system of equations of conservation of mass, momentum, and energy. The mathematic formulations for an incompressible fluid in a porous medium can be expressed as (Cathles 1977; Parmentier and Spooner 1978; Turcotte and Schubert 2002):

$$\nabla(\rho_f U) = 0 \quad (12)$$

$$U = -\frac{k}{\mu_f}(\nabla P + \rho_f g) \quad (13)$$

$$\rho_b C_b \frac{\partial T}{\partial t} = \lambda_b \nabla^2 T - (\rho_f C_f U T) + Q \quad (14)$$

where T is temperature, t time, ρ density, C specific heat, λ conductivity, U Darcy velocity, Q internal heat source, P pressure, k permeability, μ dynamic viscosity and g the acceleration of gravity, and subscript f denotes fluid property, and b bulk (rock + fluid) property. Equation (12) represents conservation of mass flow of the fluid, Equation (13) is conservation of momentum expressed by Darcy's law. Equation (14) represents conservation of energy where rock and fluid are assumed to be in local thermal equilibrium at temperature T . The system of equations is solved using an explicit finite difference scheme.

Reconstruction of exhumation histories of igneous bodies. The reconstruction of exhumation histories of igneous bodies is achieved by determining the emplacement states of igneous intrusions and calculating the erosion rates for both the country rocks and igneous rocks. The calculation of erosion rates is mainly based on the input thermochronometer data, whereas the emplacement depth and eroded thickness of the igneous body are determined through inverse modeling using an iterative "trial and error" strategy. For detailed algorithms and an example of the application of 4DTHERM see Appendix II of McInnes et al. (2005b).

Currently, 4DTHERM can support the modeling of regular and irregular shapes of igneous bodies and of multiple intrusion events. It is possible to produce a unique solution to the emplacement depth and eroded thickness of igneous units through the use of multiple geochronology datasets (i.e., each sample containing three or more thermochronology ages) from multiple sample locations in the same igneous unit.

4DTHERM inputs

Data inputs to the model include: (1) size and shape of igneous and country rock units; (2) residual sizes, position, and properties of igneous bodies; (3) age data and corresponding nominal closure temperatures, and (4) sample position. The construction of geologic bodies (including country rocks and igneous rocks) can be done either through the "Geobody Building" panel (for regular shapes only), or by drawing directly on the model using the mouse (for both regular and irregular shapes) (Fig. 19). Alternatively, these input data can be loaded separately from formatted text files.

4DTHERM provides a default geologic background initialized with a set of initial parameters (e.g., surface temperature, thermal gradient, basal heat flow, lithology, thermal conductivity, specific heat, and density, etc.), which can be edited using the "Parameter Settings" panel.

4DTHERM outputs

The outputs available after each successful test include: (1) digitized cooling curves with highlighted key points (Fig. 20); (2) parameters calculated during the modeling run such as

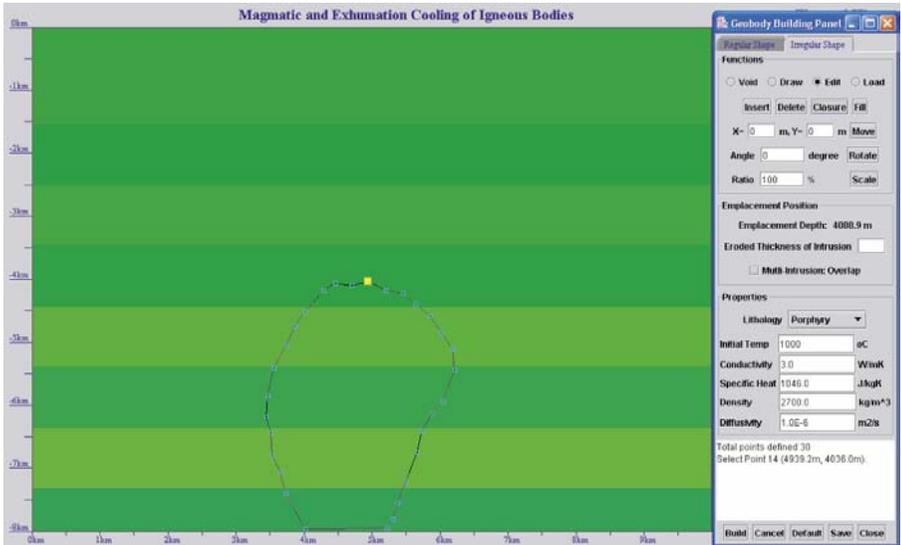


Figure 19. An example showing the construction of an igneous body by mouse drawing. The igneous body drawn on the cross section can be resized, scaled and rotated through the Geobody Building Panel on the right. The properties of the igneous body can be assigned via the input text fields in the panel.

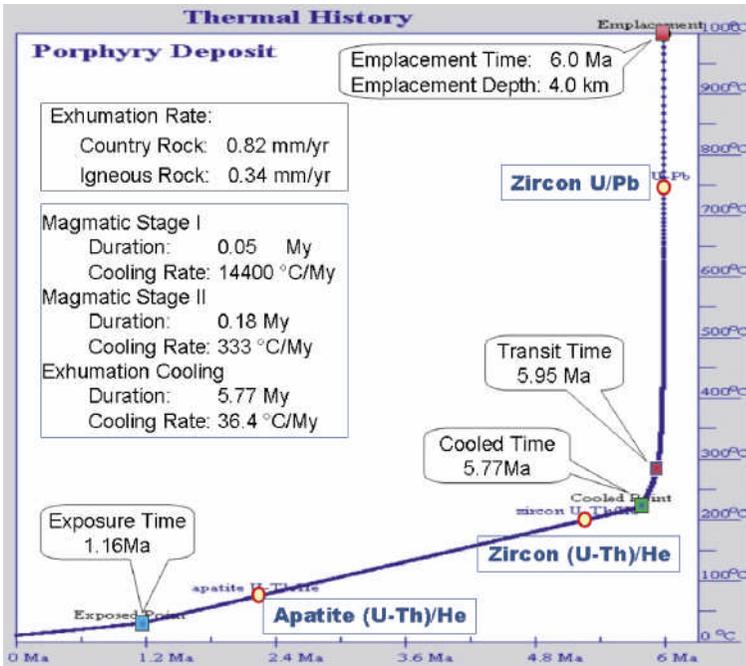


Figure 20. Example showing the output available in a successful modeling case. The modeled cooling curve for an igneous body matches all three age data (small red circles). Some critical time points are highlighted by small colored rectangles. Cooling rates, exhumation rates and many other parameters can be calculated based on the digitized cooling curve.

depth and time of emplacement, cooling rates of different stages, exhumation/erosion rates for country rocks and igneous rocks, eroded thicknesses of intrusions, and the exposure time if the sample was exhumed to the surface; (3) detailed step-by-step modeling states. These data can be saved in formatted text files for further examination. In addition, the instant visualization of temperature distribution in the 2D model at each time step is another source of output and can be saved using "Print Screen" button on the keyboard.

CONCLUDING REMARKS

The computational tools presented in this chapter (Table 1) are useful for simulating processes on a variety of temporal and spatial scales. Crustal and magmatic thermal processes can be simulated with the 4DTHERM RESPTIME, AGE2EDOT, and TERRA programs. Simulation of fission track annealing and analysis of track length distributions are possible with HeFTy, FTIndex, TASC, BINOMFIT, CLOSURE and TERRA programs. And finally, prediction of (U-Th)/He ages is possible with HeFTy, DECOMP, and TERRA programs. Future applications of thermochronometer data to different geologic problems will hopefully benefit from the continued development and free distribution of programs such as these. New directions of thermochronometer related software development will hopefully focus on not only implementing new and improved kinetic models for different thermochronometer systems, but also on relating different geologic processes (e.g., landscape evolution, shear heating on faults, etc.) to testable scenarios of predicted thermochronometer ages.

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