HeFTy
Beta version 2

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1. Installation

1.1. Hardware and Software Requirements

HeFTy is written for the Microsoft Windows operating system. It was developed in Borland C++ Builder version 6.0. It should work on all current versions of Windows, including Windows 2000 and XP. There are no minimum hardware requirements (it will run on any computer capable of hosting Windows), but the inversion functions are very processor intensive, so faster processors will result in faster inversions.

1.2. Program Installation

In most cases, HeFTy is distributed as a self-extracting ZIP archive. Double-click on the archive file, and you wil be prompted for where to unload the files. The default is C:\Program Files\HeFTy. After you select a directory, all necessary files will be unpacked to that directory.

HeFTy requires several libraries to run, including: BORLNDMM.DLL, CC3260MT.DLL, RTL60.BPL, STLPMT45.DLL, and VCL60.DLL. These files will be automatically unpacked into the program directory; however, they can also reside in Windows system folders, such as \Windows\System32.

1.3. File Naming Convention

The file types cited in this manual (HFT) are recognized by the Windows operating systems based on their extension consisting of these characters (i.e., an HFT file must end in ".HFT" or ".hft"). HeFTy will only read files with proper extensions.

1.4. The HEFTYPREFS.DAT File

The first time HeFTy is run, it creates a file HEFTYPREFS.DAT in the same directory where the executable program resides. This file contains certain information that may be specific to individual users, including their calibrations for initial fission-track length and length reduction observed in measurement of a standard, preferred (U-

Th)/He systems and their calibrations, etc. This file is automatically maintained by HeFTy, and cannot be edited by hand; all calibrations are entered through the normal program interface. If the HEFTYPREFS.DAT file is ever deleted or corrupted, HeFTy will generate a new one with the default settings. If this happens, users may have to re-enter their calibration information.

If there are multiple users of HeFTy, each with their own calibrations, a separate copy of the program should be made for each one, and kept in separate directories, so that separate HEFTYPREFS.DAT files will be maintained for each.

2. Program Interface and Overview

2.1. Introduction

HeFTy was created to help the geologist to obtain the maximum amount of information possible from thermochronometric and related data through forward and inverse modeling. The program is designed around a graphical user interface to make data entry and thermal history generation easy and intuitive. This chapter describes the main features of the interface.

2.2. The Main Program Window

2.2.1. General. HeFTy uses a "multiple document interface," similar to many other Windows programs. It has a main program window, within which zero, one, or more document files may be open. Each document file corresponds to a single sample or locality, which can have associated with it one or more thermochronometers. Figure 2-1 shows an example screen from HeFTy, with one file window open.

The main program window contains the menus and "speed buttons" that enable most program operations. The buttons replicate the most-used commands, which are all available from the pull-down menus as well. Each button is described in detail below. The buttons and corresponding menu commands are automatically grayed out when they are not available.

2.2.2. "New blank model" button. This button creates a new model with no thermochronometers preloaded into it. Thermochronometers can be added with the "+" button, discussed below (2.2.5).

2.2.3. "New AFT model" button. This button creates a new model with a single apatite fission-track thermochronometer added.

2.2.4. "New (U-Th)/He model" button. This button creates a new model with a single (U-Th)/He thermochronometer added.

2.2.5. "Open file" button. This button brings up a dialog for opening a HeFTy model file. HeFTy file names have the extension ".hft".

2.2.6. "Save file" button. This button brings up a dialog allowing the current file window to be saved. HeFTy files have a specialized format that is only readable by HeFTy. They must end in the extension ".hft".

2.2.7. "Add thermochronometer" button. When this button is pressed, a menu pops up listing the thermochronometers that can be added; choose the appropriate item to add it to the currently top-most model window. Up to seven thermochronometers can be added to any model. Duplicate thermochronometers are allowed.

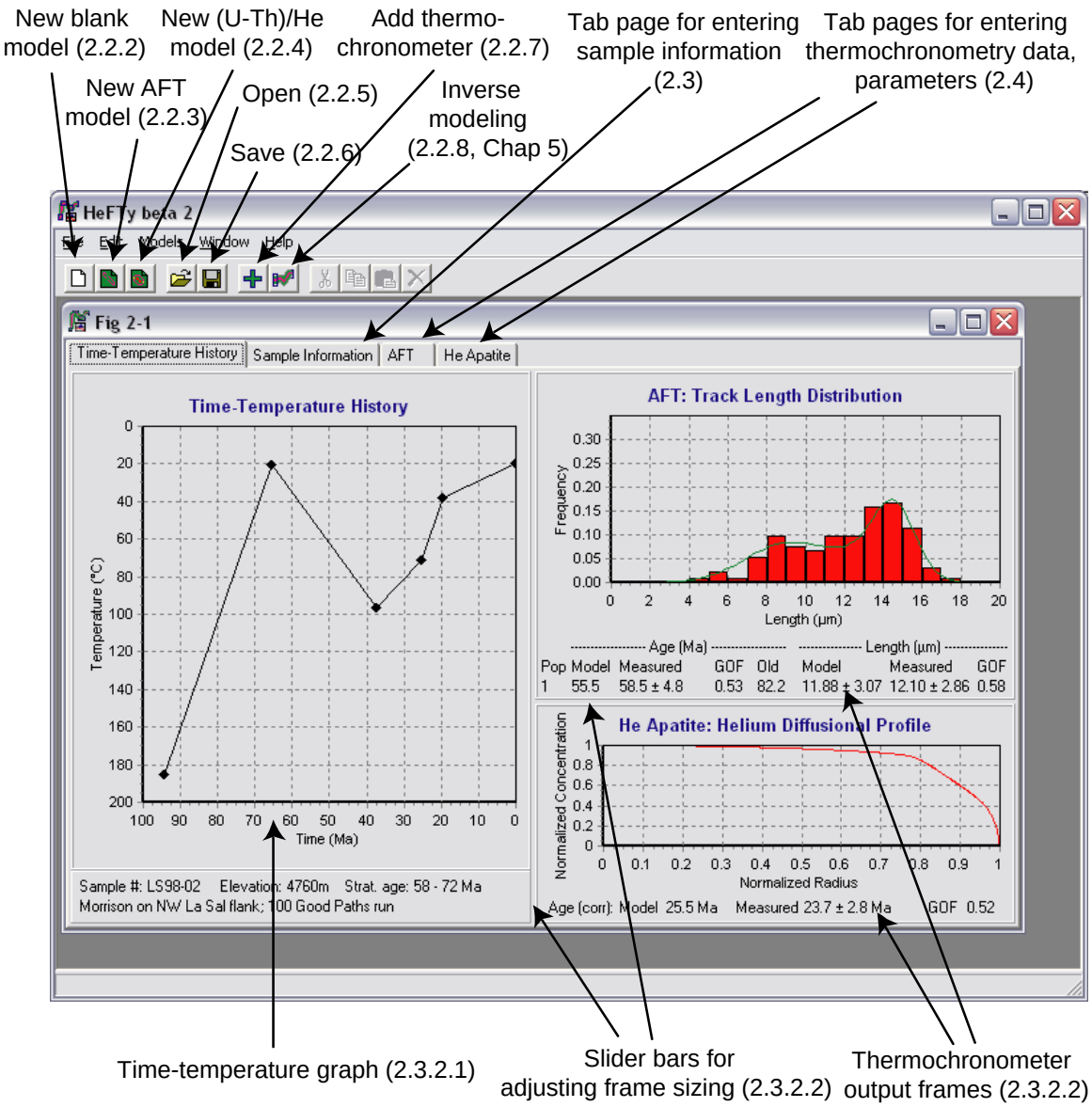

Figure 2-1: Main program window, with one model file open.

2.2.8. "Inverse modeling" button. This button brings up the window that enables inverse modeling. Inverse modeling is discussed in Chapter 5 of this manual.

2.3. Model (File) Windows

2.3.1. General. The model windows use tabbed pages to provide easy access to all of the information about a sample and the thermochronometers used to characterize it. The first two tabs are always the same ("Time-temperature history" and "Sample Information"), and for each thermochronometer added to the model another tab is created. Clicking on a tab marker brings the corresponding tab page to the front of the window.

2.3.2. Time-Temperature History tab page. An example of this tab page is shown in Figure 2-1. The page is divided into multiple sections, with different sections separated by slider bars. The relative sizes of each window section can be changed by clicking and dragging on the slider bars.

2.3.2.1. Time-temperature graph. The top left section always shows the time-temperature history graph. This window can be used for creating forward model time-temperature histories by clicking and dragging with the mouse. Clicking on a blank part of the graph adds new point to the time-temperature path, and clicking on a pre-existing point allows it to be dragged. One or more points can be deleted by right-clicking in the graph, which brings up a pop-up menu listing the options available.

Double-clicking on a graph axis brings up a dialog (Fig. 2-2) allowing various aspects of the axis to be changed, including the maximum value, the spacing between labels, and the visibility of the dotted-line grids.

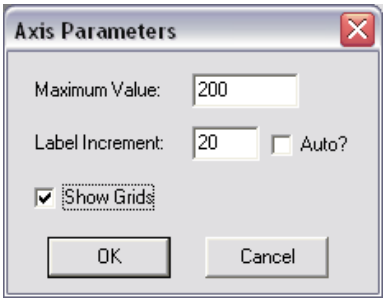

Figure 2-2. Dialog for adjusting graph axis parameters.

Below the time-temperature path are some sample information is shown; this information is entered in the "Sample Information" tab page (2.3.3).

2.3.2.2. Thermochronometer output frames and slider bars. If the model has no thermochronometers added to it, the time-temperature graph takes up the entire tab page. When thermochronometers are added, new sections are added to the page. Each new section contains the output results for a thermochronometer; these are called *output frames*. For example, for the apatite fission-track thermochronometer, the output frame contains the measured and modeled track length distribution and age, and statistics

reflecting the degree of matching between them. By clicking and dragging points in the time-temperature graph, the user can immediately see how this changes the predictions for the model results and the goodness of fit between model and data. The gaps between the different sections are actually slider bars, which allow the relative sizes of the windows to be changed by clicking and dragging.

2.3.3. Sample Information tab page. An example of this page is shown in Figure 2-3. This page allows information about the sample to be recorded, including sample number, description, stratigraphic age, elevation/depth, and any notes the user wishes to save concerning the sample or its analysis. At present, nothing is done with this information; however, future versions of the program may use some of this information to aid in analysis.

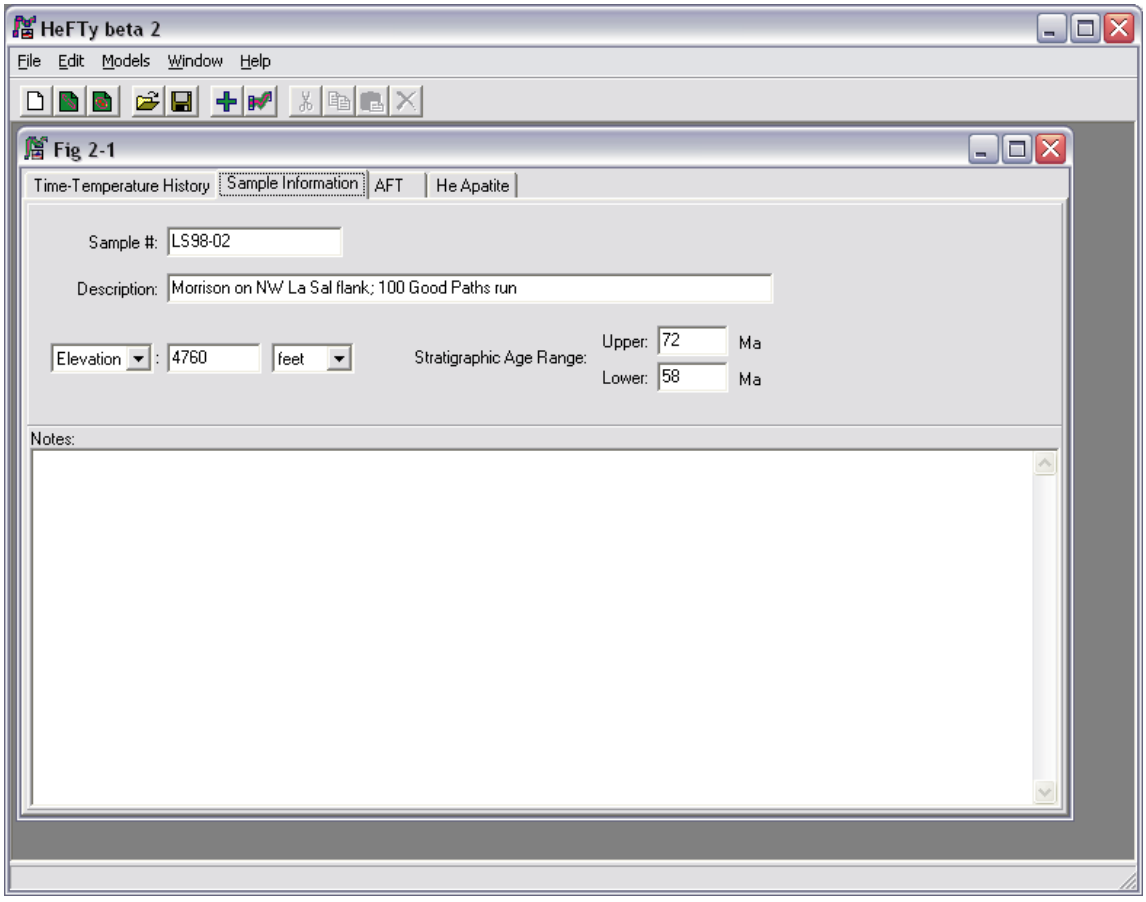

Figure 2-3: The *Sample Information* tab page.

2.3.4. Thermochonometer tab pages. Each instance of a thermochronometer added to a model will have an output frame on the Time-Temperature History tab page,

and its own tab page for entry of system parameters and/or data to be fitted. The tab pages for each thermochronometer are discussed in detail in Chapter 3.

Thermochronometers can be deleted from a model by right-clicking on their page tab, and selecting the "Delete…" option from the pop-up menu. The pop-up menu also allows the tab to be renamed.

2.4. File Formats

In addition to typing and cut-and-pasting, many types of data can be entered into HeFTy using tab-delimited text files. A set of example files is found in the Microsoft Excel file accompanying the HeFTy distribution, "Import Templates.xls". These file formats are also described in Appendix A.

HeFTy saves model files in a binary format that is only readable by HeFTy, unlike old AFTSolve files that were readable text. HeFTy files have the extension ".HFT" or ".hft".

2.5. Exporting Graphics

All graphs that appear in HeFTy can be exported to other programs by right-clicking on the graph and choosing one of the "Copy" options:

- *Copy as bitmap*: This copies the pixel image of the graph to the Windows clipboard, so it can be pasted into many programs (Word, PowerPoint, Photoshop) as a pixel image. The graph is just a pixel image, which is sufficient for reports or presentations, but not for most formal publications.
- *Copy as WMF*: This makes a "Windows metafile" version of the graph and copies it onto the clipboard. If pasted into a graphics program such as Adobe Illustrator, it is transferred as a set of graphics objects (lines, shapes, text, etc.) that can be edited directly. If pasted into Microsoft Word, when resized line thicknesses and fonts are automatically adjusted as well (although sometimes it can look slightly unusual on the computer screen).

3. Thermochronometric Systems

3.1. Introduction

HeFTy was designed to allow simultaneous calculation of multiple thermochronometric systems describing a single sample or locality. Thermochronometric systems currently included are apatite fission track, (U-Th)/He, and vitrinite reflectance. Apatite fission-track calculations can use the models of Ketcham et al. (1999), Laslett et al. (1987), and Crowley et al. (1991). The (U-Th)/He calculations permit modeling of any mineral for which the appropriate kinetic data have been determined, such as apatite, titanite and zircon (e.g., Farley, 2000; Reiners and Farley, 1999; Reiners et al, 2004). Vitrinite reflectance is modeled using the EasyRo% method of Sweeney and Burnham (1990). The modular design of HeFTy allows for incorporation of additional thermochronometers in the future, such as zircon fission track.

This chapter reviews the thermochronometric systems in the program, and how model parameters and data are entered.

3.2. Apatite Fission-Track System

3.2.1. Background. Apatite fission track (AFT) thermochronology is based on the accumulation of structural damage in an apatite crystal due to the fission decay of ^{238}U atoms. The fission particles leave damage trails, which can be detected by polishing a cross section of a crystal and etching it with an acid. In general terms, the fission-track density, or number of fission tracks per unit area, reflects the time elapsed since the crystal last cooled sufficiently to retain fission damage, and the fission track lengths reflect the temperatures that the crystal has experienced. In most apatites, fission damage anneals over geological time scales at temperatures above ~110°C, but some apatites with unusual (but not necessarily rare) compositions retain their tracks at much higher temperatures (Ketcham et al., 1999). This process is referred to as kinetic variability, as the effect of these variations is to affect the apatite annealing kinetics. For a comprehensive overview of the apatite fission-track system, see Donelick et al. (2005) and Ketcham (2005b).

3.2.2. Kinetic data. Incorporation of some kind of kinetic data is often crucial for valid interpretation of apatite fission-track data. In the vast majority of sedimentary rocks, the apatites from a sample have a range of kinetic behaviors (i.e. different

resistance to annealing over geological time scales). The averaging effects of lumping all of these apatites into one group may obscure both the timing and temperature information potentially discernible from fission-track analysis. By sorting and separating apatites into kinetic populations, not only is the reliability of the analysis increased, but the power as well, as multiple kinetic populations simultaneously constrain the thermal history of the sample in different ways.

One of the principal features of HeFTy is its ability to deal with apatites that have a range of kinetic behaviors. D_{par} and Cl content are two routinely used parameters that, in many cases, exhibit a strong and informative correlation with apatite fission-track ages and lengths. D_{par} is the mean fission-track etch pit diameter parallel to the crystallographic *c*-axis for each apatite grain, and is specified in units of microns (e.g., Donelick, 1993; Donelick, 1995; Carlson et al., 1999). Cl content is expressed in the Ketcham et al. (1999) model in terms of atoms per formula units (apfu or pfu), based on a two-anion unit cell and a complete stoichiometric analysis of apatite using an electron microprobe; because many workers use weight percent rather than apfu, an weight-percent-based version of this model is also included in HeFTy. Ketcham et al. (1999) also presented a model based on OH pfu content. In addition to these variables, other, less frequently encountered cation substitutions (Fe, Mn, Sr, REE's) can also change annealing behavior.

Collectively, we say that D_{par}, Cl, and OH are good potential indicators of fission-track annealing kinetic properties among natural apatite grains. Experience shows that any of these parameters gives essentially the same result in most cases (e.g., Burtner et al., 1994). The default kinetic variable used by HeFTy is D_{par}. Use of this parameter for interpretation of apatite fission-track data is patented by Raymond A. Donelick (U.S. Patent Number 5.267,274 and Australian Patent Number 658,800), and restrictions on use are specified in the **Copyright/Licensing Notice** at the beginning of this manual. Observed values in nature of D_{par} range from approximately 1.50 μm for apatites that are least resistant to annealing to approximately 5.00 μm or higher for apatites that are often most resistant to annealing. Either Cl pfu and OH pfu may also be selected as the kinetic parameter. Observed values in nature of Cl pfu range from approximately 0 pfu for apatites that are least resistant (unless there are other significant cation substitutions) to 2 pfu for endmember Cl-apatite; resistance to annealing increases from 0 pfu until approximately 1 pfu, after which the relationship becomes unclear. OH pfu also ranges from 0 to 2 in nature and it appears to be correlated with Cl pfu, but it is unclear how to generalized resistance to annealing in terms of OH pfu.

HeFTy quantitatively relates D_{par}, Cl and OH to annealing behavior by using them to calculate a variable called r_{mr0}, which is defined by Ketcham et al. (1999). Values for r_{mr0} span the range from 0 to about 0.87, with high values being typical of most apatites with low annealing resistance, and low values indicating high resistance to annealing, or high closure temperatures. Because resistance to annealing can also be affected by other compositional variables, HeFTy also allows direct input of r_{mr0} into the model for expert users who wish to estimate this variable using additional data.

As currently written, the D_{par} calibration used in this program is only valid for etch pit data measured by Raymond A. Donelick (all apatites etched for 20 seconds at 21°C in 5.5N HNO_3). If D_{par} data from another worker are to be used, it is necessary for

that worker to calibrate D_{par} values to the various annealing models. If such a calibration is done, it can be included in the program using the AFT Preferences page (see Chapter 5).

3.2.3. Length measurement considerations. In almost all cases, fission-track length measurements are made on confined, horizontal tracks; i.e. tracks interior to the crystal, where both ends can be seen, and parallel to the cut surface of the crystal. Usually, this cut surface is along a prismatic face, and the apatite *c*-axis is in the plane of the section. Fission-track lengths are anisotropic, in that, for a given level of annealing, tracks parallel to the *c*-axis tend to be longer than tracks that are perpendicular; this anisotropy increases with increasing level of annealing.

Although long taken for granted, the repeatability of fission-track length measurements has been receiving increased research attention of late. Barbarand et al. (2003) documented numerous instances in which the uncertainty in the mean track length exceeded the expectation from traditional statistical analysis. There is no agreed-upon cross-calibration regime for fission-track length measurements, aside from measuring natural lengths in some apatite standards (Durango, Fish Canyon), which is of positive but limited value.

HeFTy includes two features intended to increase the reliability of length data: initial length calibration and *c*-axis projection.

Initial track length, or the assumed length of tracks before the onset of annealing, varies as a function of etching technique and apatite etching properties (Carlson et al., 1999). The range of mean initial track lengths among the 15 apatites studied by Carlson et al. (1999) was about 1.2 µm; a 0.6 µm divergence in initial length can affect estimates of degree of unroofing by several hundred meters. Initial track length is well-correlated with D_{par}, and somewhat correlated with Cl content, and thus these measurements can be used to improve the accuracy of the initial track length estimate. HeFTy allows initial track length estimates to be imported along with length measurements, and alternatively offers means to make these estimates within the program.

C-axis projection is a method for correcting for track-length anisotropy effects and taking angular information into account by estimating the length that each track would have if it were in a *c*-axis parallel orientation. This procedure removes a lot of noise from the length data, and is likely to remove some degree of inter-operator bias (Ketcham 2005a).

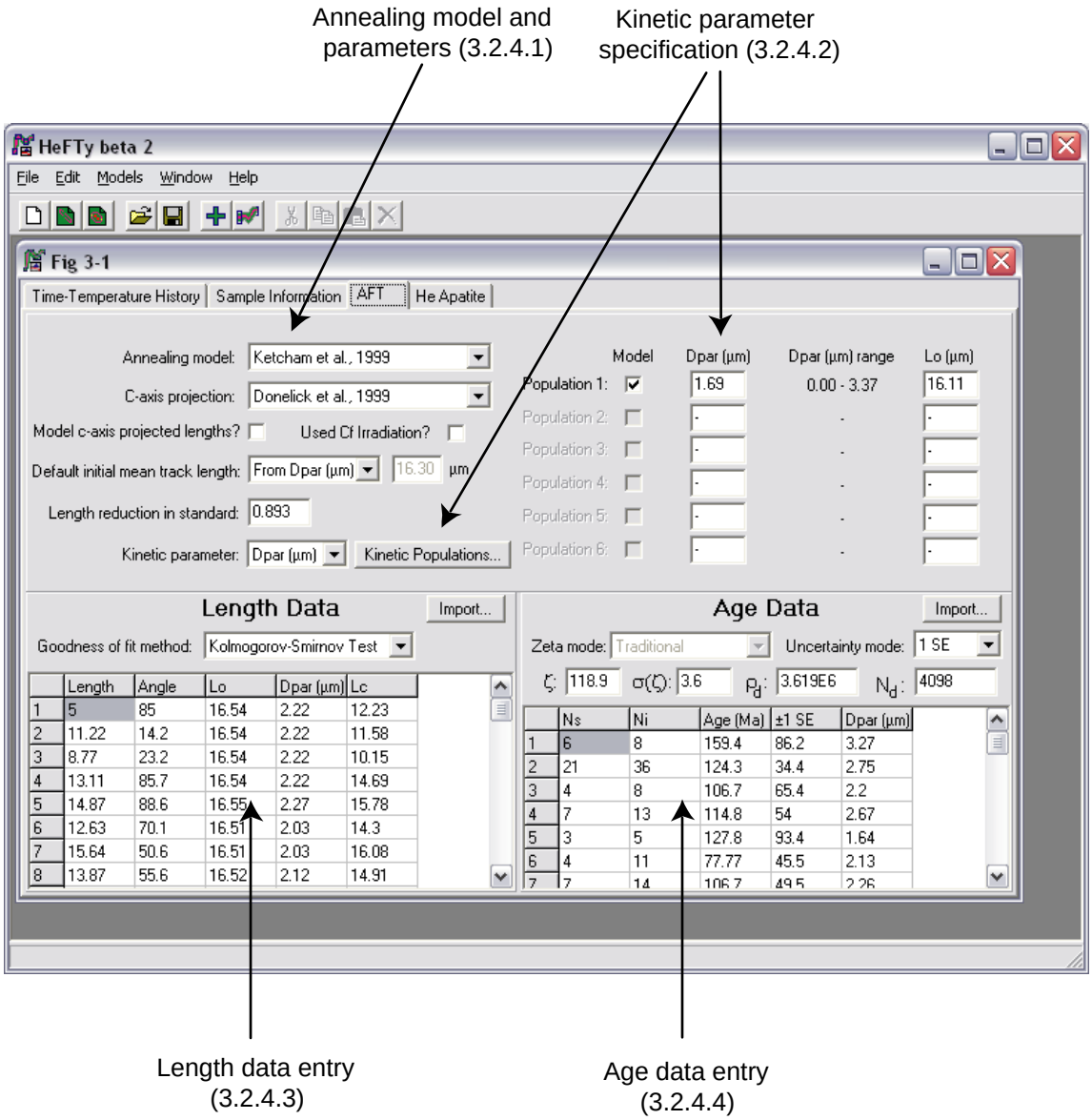

Figure 3-1: The AFT data and parameter entry tab page

3.2.4. The AFT input tab page. Figure 3-1 shows the tab page that is generated for each AFT thermochronometer. The upper part of the page is predominantly concerned with model parameters, and the bottom is for data; however, there is some crossover, as the program includes some features that reconfigure model parameters to match the data. Each section will be discussed individually.

3.2.4.1. Annealing model and parameters. This section allows the user to set up the primary controls for how calculations are done.

- *Annealing model*: This drop-down list allows the user to specify which fission-track annealing calibration will be used to calculate track length reduction as a function of time and temperature. Three models are currently

supported: Laslett et al. (1987) for Durango apatite, Crowley et al. (1991) for F-apatite, and the Ketcham et al. (1999) multi-kinetic model.

- *C-axis projection*: Two projection models are available: Donelick et al. (1999) and Ketcham (2003). This parameter only has an effect when the Ketcham et al. (1999) annealing model is used, and the "Model c-axis projected lengths?" box is checked.
- *Model c-axis projected lengths?*: Check this box to generate track length histograms using of c-axis parallel (rather than randomly oriented) track lengths. This function is only available if the Ketcham et al. (1999) annealing model is being used.
- *Used Cf irradiation?*: This box should be checked if working with track length measurements acquired with the aid of Cf irradiation, which enhances detection of horizontal confined tracks (Donelick and Miller, 1991).
- *Default initial mean track length*: This allows the user to set the assumed initial (unannealed) track length as either a constant or a function of one of the kinetic variables. If a constant, all tracks are assumed to have the same initial length, which is entered into the adjacent text box. If a function, an initial length estimate is generated for each length measurement based on its corresponding kinetic parameter value. The default functions relating initial length to mean kinetic parameter are from Carlson et al. (1999); these functions can be customized for users' own calibrations on the AFT Preference page (Chapter 5).
- *Length reduction in standard*: This is the ratio of spontaneous track length to induced track length in the standard used for calibration, usually Durango apatite.

3.2.4.2. Kinetic parameter specification. Kinetic parameters are added using the bottom two controls in the left column in the upper portion of the tab page, and the sequence of controls on the right. These aspects of HeFTy only have meaning if the Ketcham et al. (1999) multi-kinetic annealing model is used. HeFTy implements multi-kinetic AFT modeling by allowing up to six monokinetic populations to be defined, either based on the length and single-grain age data using the "Kinetic Populations" function, or explicitly by typing in values in the six sets of controls in the right-hand column.

The "Kinetic parameter" drop list allows the user to specify which kinetic variable (D_{par}, Cl, OH, r_{mr0}) will be used to distinguish different populations. If the user imports data with a kinetic variable, this box is set automatically.

The "Kinetic Populations" button brings up a dialog box (Figure 3-2) that allows lengths and single-grain ages to be separated into monokinetic populations to be modeled separately but in parallel. Populations are separated by dividers, which can be added to the graph by clicking in it. Clicking and dragging on a divider moves it. As a divider moves, HeFTy calculates the pooled single-grain age mean length of each population, and evaluates the chi-squared test for the single-grain ages to test whether they could have been drawn from the same kinetic population. Populations that pass the chi-squared test have their ages shown in blue regular type, while populations that do not pass chi-

squared have their pooled ages shown in red italics. Only populations that pass the chi-squared test should be modeled. To toggle whether a population is modeled or not, right click in its region of the graph, and choose the "Toggle population" menu option. Populations omitted from modeling are shaded in light red. In the example shown in Figure 3-2, five population are defined, of which three will be modeled and two omitted. The first population consists of a single grain with no corresponding Dpar measurement.

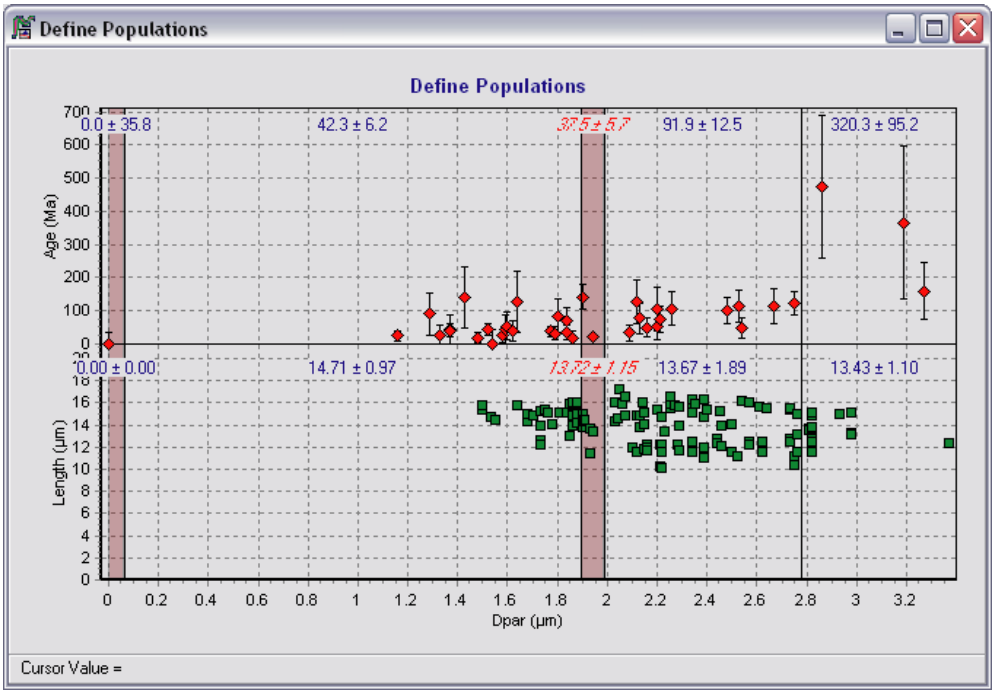

Figure 3-2: The "Define Populations" dialog

The populations defined in this dialog correspond to the six sets of controls on the right side of the AFT tab page. As population boundaries are changed by the user, these controls are automatically updated as well. Each population has an on/off check box, and characteristic (mean) kinetic parameter value, and an estimated initial track length.

3.2.4.3. Length data entry. The lower left hand portion of the AFT tab page is used for entering track length data. The three ways to enter data, in order of increasing difficulty are: importing it using a tab-delimited text file; cut-and-pasting it from a spreadsheet application, such as Microsoft Excel; and typing it directly into the program. The available file formats for importing length data are discussed in Appendix A, and examples are provided in the Excel file "Import Templates.xls", which is provided with HeFTy.

3.2.4.3.1 Goodness of fit method: This drop list is used to control the function that is used to compare measured length histograms to model results. The two options are the Kolmogorov-Smirnov Test, and Kuiper's Statistic (Press et al., 1992). The Kolmogorov-Smirnov test is most sensitive at about the median track

length value in a distribution, whereas Kuiper's statistic equalizes sensitivity between the median and tails.

3.2.4.3.2. Length spreadsheet. The length data columns are:

- *Length (in micrometers)*: The length of an individual fission track.
- *Angle (in degrees)*: The angle of that track to the crystallographic c-axis. This is only used if *c*-axis projection is employed; if there are no angular data, just enter "0" in this column.
- *Lo (in micrometers)*: The assumed initial (unannealed) length of this fission track. This value can either be entered by the user, or it can be generated by the program according to the "Default initial track length" setting when importing from a tab-delimited text file.
- *Kinetic parameter (D_{par}, Cl, OH, r_{mr0}; units as appropriate)*: The kinetic parameter associated with this fission track.
- *Lc (in micrometers)*: The *c*-axis projected length of this fission track. This value is calculated and maintained automatically by HeFTy; once the rest of the data are complete for a track, HeFTy calculates and fills in the value. The Lc column is automatically updated whenever the other data for a track (length, angle, Lo) are added, deleted or altered.

Values can also be cut-and-pasted out of this area and into a spreadsheet or word processing program. Simply highlight the region desired by clicking on the mouse and dragging, and then either right-click to access a pop-up menu, or use the "Cut" or "Copy" options in the Edit menu to transfer the data to the Windows clipboard, after which it can be pasted into any program that will accept it.

***3.2.4.4 Age data entry*.** The lower right hand portion of the AFT tab page is used for entering single-grain age data. In general, HeFTy requires the "raw" data for each grain, and the associated calibration parameters. There are a number of options in HeFTy for how age and uncertainty calculations are handled, described below.

3.2.4.4.1. Age calculations. HeFTy supports three age calculation methods, described below. Because they require different data, if any data are present in the spreadsheet the age calculation method setting cannot be changed; the only way to change this setting is by deleting all spreadsheet data. The age calculation methods, and their required calibration parameters and data, are

- *Traditional*: The traditional zeta calibration method fission-track age determination (Hurford and Green, 1983). This method requires values for zeta (ζ), uncertainty in zeta ($\sigma(\zeta)$), measured fission-track density in a standard dosimeter glass (ρ_d), and total number of track measured in the glass (N_d). The data required for each grain are the spontaneous and induced track counts (N_s and N_i, respectively), and optimally a kinetic parameter value.
- *Phi method*: This method, from Jonckheere (2003), is an attempt to bypass the need for an age standard by instead utilizing a neutron fluence measurement (ϕ,$\sigma(\phi)$) in combination with an alternative zeta formulation that mainly

quantifies geometric factors (ζ,$\sigma(\zeta)$). As with the traditional zeta method, the data required for each grain are the spontaneous and induced track counts, and an additional kinetic parameter is strongly encouraged. Some details of the phi method ad implemented in HeFTy are discussed in Appendix D.2.

- *LA-ICPMS ratio*: This method (Donelick et al., in revision) uses laser ablation inductively coupled mass spectrometry to measure U in grains, rather than the external detector method. The only calibration parameters required are a zeta value and its uncertainty (ζ,$\sigma(\zeta)$). For each grain, this method requires the spontaneous track count, the area over which spontaneous tracks were counted, an isotopic ratio measured on that grain (for example, $^{43}Ca/^{238}U$; denoted P_{corr}) and its uncertainty ($s(P_{corr})$), and, optimally, a kinetic parameter.

As with length data, age data can be entered by means of a tab-delimited text file (described in Appendix A, with examples in "Import Templates.xls"), by cutting-and-pasting from a spreadsheet, or by typing directly into HeFTy.

3.2.4.4.2. Uncertainty modes. HeFTy supports a number of different methods for calculating, presenting, and working with the uncertainty in fission-track ages. Although most age determinations are presented as a single value with a symmetrical error (e.g., 1- or 2-σ), the Poissonian statistics that are considered to best describe fission-track dating indicate in many cases that uncertainties are strongly non-symmetric, particularly with young ages. This distinction, and the equations behind it, is reported in more detail by Ketcham (2005b). The methods implemented are:

- 1 SE: Uncertainties are symmetric, and 1 standard error is reported.
- 2 SE: Uncertainties are symmetric, and two standard errors are reported (i.e. the 95% confidence limit).
- 95% +/-: Uncertainties are asymmetric, and the 95% confidence limit is reported as a positive and negative deviation from the calculated age.
- 95% int.: Uncertainties are asymmetric, and HeFTy reports the 95% confidence limit as an interval from a minimum to a maximum age.

This setting can be changed at any time; however, inversion is affected by whether the uncertainty is considered as symmetric or asymmetric, so changing this value may make the inversion inconsistent with the uncertainties as reported in this table. The columns with the single-grain uncertainties are automatically maintained, as long as all of the data and calibration parameters have been entered.

3.2.5. The AFT output panel. Figure 3-3 shows a pair of examples of the panel that appears on the Time-Temperature History tab page for an AFT thermochronometer. The left panel shows a typical mono-kinetic model, and the right panel shows a multi-kinetic model, following the division of data into kinetic populations shown in Figure 3-2.

In both cases, the track length data are shown as solid red histograms, and the calculated track length distributions based on the current time-temperature path are

shown as dark green lines. In the multi-kinetic case, the histograms for each population are stacked, with the ordering corresponding to the order of populations defined in the AFT data (Fig. 3-2); the y axes are labeled with the appropriate population numbers. Note that not only data but model results differ among these cases, as each population is modeled with a different annealing equation to reflect the inferred change in annealing kinetics.

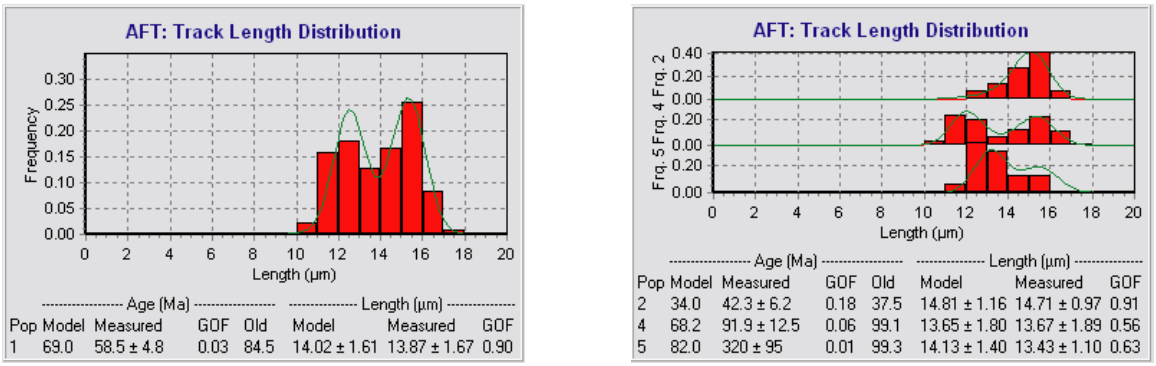

Figure 3-3: Example AFT output frames.

Below the histograms are sequences of numbers describing the model and data and how well they match. There is one line for each population being modeled. After the population number, the first set of values describes the model-calculated age, the data calculated age and uncertainty (according to the uncertainty mode selected; see 3.2.4.2), and goodness of fit ("GOF"). The goodness of fit indicates the probability of failing the null hypothesis that the model and data are different. In general a value of 0.05 or higher is considered not to fail the null hypothesis, and thus reflects an acceptable fit between model and data. Statistics are discussed in more detail in Chapter 5. After the age GOF is the age of the oldest fission track that has not fully annealed ("Old"); this corresponds to the earliest time in the thermal history that is in any way constrained by fission-track data. The next set of numbers describes the mean lengths of the model and data, the standard deviations of the length distributions, and their goodness of fit.

3.3. (U-Th)/He System

3.3.1. Background. (U-Th)/He thermochronometry utilizes the accumulation of alpha particles (^{4}He) in a mineral due to radioactive decay of U and Th (and, in some instances, Sr or other comparatively scarce alpha-emitting isotopes). This ^{4}He can be retained within the mineral, but can also be lost by diffusion to the grain margin, which occurs as a function of temperature. In addition, because alpha particles do not stop until they have traveled on the order of 20 microns from their parent atom, some proportion of He produced near the margin will be ejected from the grain.

3.3.2. Helium diffusivity in minerals. The diffusivity of He in minerals is characterized using an Arrhenius relationship of the general form:

$$\frac{D}{a^2} = \frac{D_0}{a^2}\exp\left(-\frac{E_a}{RT}\right),$$

where D is the diffusivity, a is the radius of the diffusional domain, D_0 is the frequency factor, E_a is an activation energy, R is the Universal Gas Constant, and T is temperature (in Kelvins). In some isotopic system the diffusional domain is thought to be a small subset of a typical mineral grain, but most current studies on (U-Th)/He find that the diffusional domain is the radius of the entire grain, in which case the "*a*" terms can safely cancel each other out.

HeFTy has the currently accepted Arrhenius parameters for apatite (Farley 2000), zircon (Reiners et al. 2004), and titanite (Reiners and Farley 1999) automatically entered into the program, in addition to the older apatite model of Wolf et al. (1996), which assumes a subgrain diffusional domain. In addition, it allows the user to enter alternative Arrhenius parameters for any of these minerals, or any other mineral. The frequency term can be entered in any of four forms: D_0 or $\log_{10}(D_0)$ if the diffusion domain is the entire grain, and D_0/a^2 or $\log_{10}(D_0/a^2)$ if the diffusion domain has a smaller scale than the entire grain.

3.3.3. Alpha stopping distance effects. When an alpha particle is ejected from a nucleus, it generally does not come to a stop until it has traveled some 10-35 μm through crystalline material. When an atom undergoing alpha decay is near the edge of a mineral grain, there is a chance that the particle won't stop until it has left the grain entirely. This circumstance will lower the amount of helium in the grain, making it appear somewhat younger than it should (Farley et al., 1996).

Another consequence of long alpha stopping distances is that, in grains with a zoned or otherwise inhomogeneous distribution of U and Th, the distribution of He will be somewhat smoothed out, as He is effectively transferred from radioelement-rich regions to poorer ones. This can affect (U-Th)/He ages indirectly by altering the He gradients that are the driving force for diffusional loss.

Long alpha stopping distances are taken into account in two ways: by correcting the measured He age, and by modifying the diffusion simulation. (U-Th)/He ages are commonly corrected by dividing the measured age by the parameter F_T, the fraction of alpha particles that are not ejected from the grain, which is calculated based on the grain size (and, potentially, shape and zoning patterns). This calculation is an approximation, however, which breaks down when there is extreme zoning and/or old ages. HeFTy includes an alternative formulation that is more precise and durable under these conditions.

3.3.4. The (U-Th)/He input tab page. Figure 3-4 shows the tab page that is generated for each (U-Th)/He thermochronometer. The page is divided into three sections: the top is for model parameters, the middle s for measured data, and the bottom concerns composition and zoning, which may affect both model conditions and data corrections.

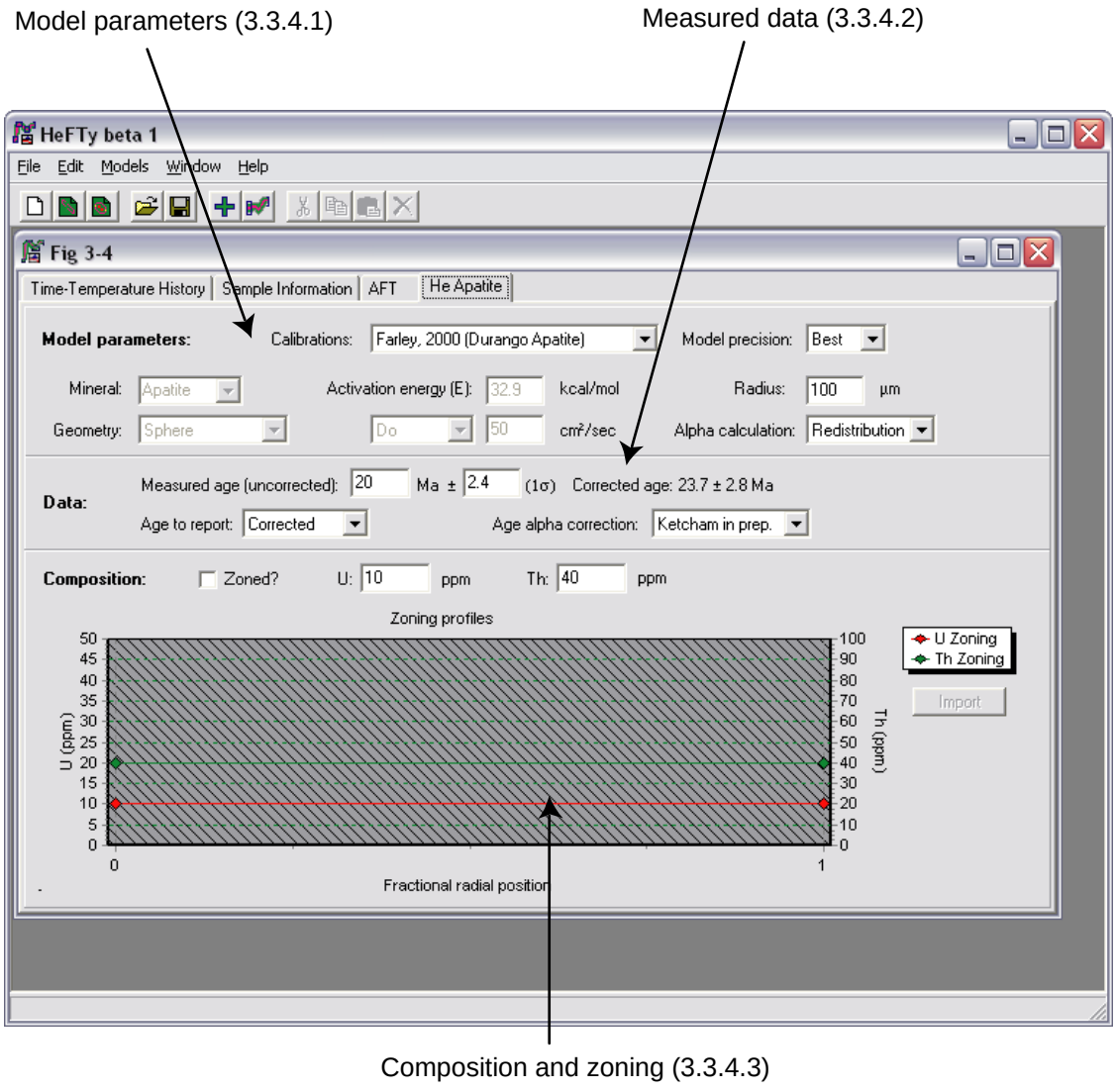

Figure 3-4: The (U-Th)/He data and parameter tab page.

3.3.4.1. Model parameters. This section allows the user to set up the primary controls for how calculations are done.

- *Calibration*: This drop-down list allows the user to choose from among several published calibrations of the kinetic properties for various minerals. If a published calibration is chosen, other parts of this section (mineral, activation energy, frequency factor) are updated automatically and dimmed, indicating that they cannot be edited. The user can also choose "Other…", which permits users to enter their own kinetic parameters.
- *Model precision*: This drop-down list controls the behind-the-scenes resources that involve trade-offs between model speed and computational precision. We recommend that the "Best" setting be used at all times, but if there are cases where speed is important (say, to make the interface run more smoothly for a class demonstration) then a lower setting can be chosen.

- *Mineral*: This drop-down list allows the user to select which mineral is being modeled. The only effect this parameter has is in calculating alpha stopping distances, which are required for age correction and incorporating alpha stopping into the model. The "Other" option can be chosen if a mineral other than apatite, zircon or titanite is chosen, but this will disable these pieces of functionality. *NOTE*: When a mineral is chosen, the title on the page tab is automatically updated, and this name appears in the (U-Th)/He output frame on the Time-Temperature History page. If "Other" is chosen, this title can be modified by right-clicking on the tab.
- *Geometry*: At this time, HeFTy simulations use a spherical grain geometry. In the future, additional geometries, such as infinite or finite cylinders, may be added.
- *Activation energy*: The activation energy for He diffusion in the mineral being modeled.
- *Frequency factor type and value*: This drop-down list and text box allow the user to specify the type of frequency factor (D_0) and its value; see section 3.3.2 for a discussion of frequency factors.
- *Radius*: This is the radius of the sphere that will be modeled. In roughly spherical grains, this may correspond to the average radius. For more elongate grains, Meesters and Dunai (2002) recommend that the radius should correspond to a sphere with the same surface-to-volume ratio (S/V) as the actual mineral grain. If one has a reasonable measurement of S/V for a grain, the appropriate radius is equal to:

$$radius = \frac{3}{(S/V)}.$$

- *Alpha calculation*: This drop-down list gives the user the options of either no correction, an ejection-only calculation, and a redistribution calculation. If the material being modeled is interior to larger grains, then "no correction" should be selected. If a grain is not zoned, the ejection-only and redistribution will give the same result; however, if zoning is included, the redistribution option should be chosen. There is no reason to ever choose the ejection-only option in practice, but it can be useful for instructional purposes to illustrate the effects of alpha stopping distances on model predictions.

3.3.4.2. Measured data. The middle section of the (U-Th)/He tab page is used for entering measured data for comparison to model results. The fields are:

- *Measured age and uncertainty (uncorrected)*: Enter the measured values, without any alpha correction. The program will automatically calculate the correction factor based on the radius entered above and compositional/zoning information below and report the corrected age.
- *Age to report*: This option allows the user to set whether the age reported by the model is corrected for alpha ejection or not.
- *Alpha age correction*: This sets the calculation used to correct ages for alpha ejection (both data age and model results). This issue is discussed further in

section 3.4.2.2. The Ketcham (in prep.) method is recommended for all situations, but the Farley et al. (1996) scheme is included for continuity and comparison purposes.

3.3.4.3. Composition and zoning. The bottom section of the (U-Th)/He tab page is for entry of compositional data for the grains being simulated. In most cases composition will have no effect on model results; the exceptions are cases where grains are zoned in U or Th, or where measured ages are very old (> ~1 Ga). Zoning can alter internal He gradients, affecting diffusion rates and potentially confounding alpha ejection corrections if not taken into account. Old ages enhance the significance of the relatively short-lived ^{235}U isotope, which affects ages and correction calculations.

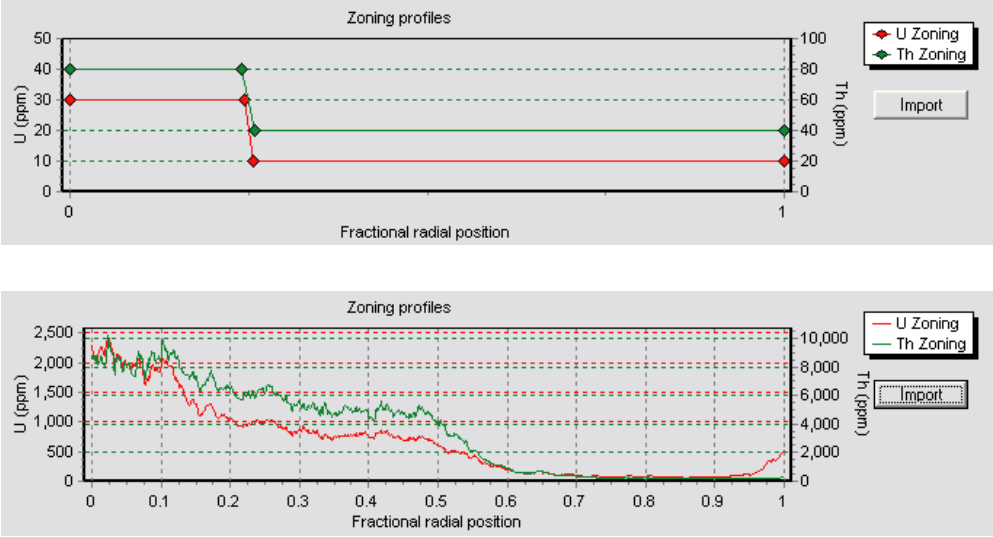

Figure 3-5. Example compositional zoning profiles. Top profile entered manually, bottom imported from text file.

The controls in the section are:

- *Zoning check box*: If unchecked, the mineral is assumed to have a uniform distribution of U and Th, with amount defined by the text controls to the right. If the box is checked, the radial distribution of U and Th are taken from the chart below.
- *U and Th (ppm)*: Use these to enter the amount of U and Th, in ppm, for a homogenous grain.
- *Zoning profiles chart*: If the zoning check box is checked, this chart is un-grayed, and allows the user to enter or import a radial zoning profile. Two examples are shown in Figure 3-5. The horizontal axis refers to fractional radial position, with the left corresponding to the grain core and the right the rim. The red line and left-hand axis refers to U concentration, and the green line and right axis refers to Th concentration. As with other graphs in HeFTy, axes can be re-scaled by double-clicking. Profiles can be entered by hand by clicking on the red or green line, which adds a nodal point that can be moved;

the end-points can also be moved, but are constrained to stay at the 0 and 1 radial positions. Alternatively, profiles can be entered from a tab-delimited text files; the format is given in Appendix A, and an example is given in "Import Templates.xls." In the upper graph in Figure 3-5, the user has entered a 2x enrichment of Th and a 3x enrichment in U in the core of the grain. The lower graph shows an example profile imported from data obtained by LA-ICPMS (data courtesy of Jeremy Hourigan and Pete Reiners).

- *Import button*: Use this button to import U and Th zoning profiles from a text file. This button is not available unless the zoning check box is checked.

3.3.5. The (U-Th)/He output panel. Figure 3-6 shows a pair of examples of the (U-Th)/He output panel as it appears in the Time-Temperature History tab page. The graphs show the radial profile of relative He concentration; from left to right corresponds to the progression from core to rim. Below the graphs are the model age, the measured age, and their goodness of fit. The left graph shows the result for an unzoned apatite grain with a radius of 66 µm with a long residence time at low temperature; the fairly sharp He profile is dominated by the effects of alpha ejection, only slightly modified by diffusion. The right graph is for the same sized grain and thermal history, only with the U and Th zoning profiles illustrated in the lower part of Figure 3-5. Here the He distribution is dominated by the radioelement zoning.

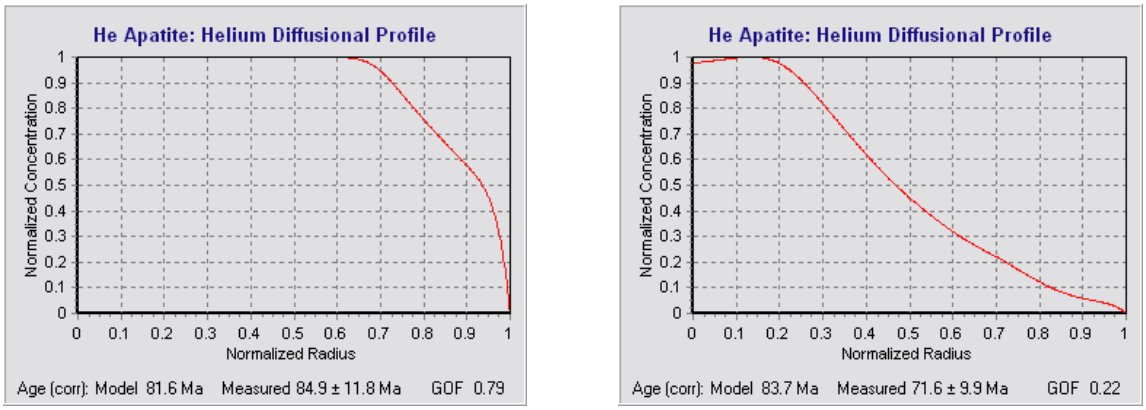

Figure 3-6: Example (U-Th)/He output frames.

3.4 Vitrinite Reflectance

3.4.1 Background. Vitrinite reflectance (%Ro) is a widely used tool for thermal history evaluation. Vitrinite is one of the primary components of coals and other organic matter found in sedimentary rocks; it forms by thermal alteration of cellulose and lignin in plant cell walls. As it is heated, its reflectance increases. Vitrinite reflectance thus records the maximum temperature that a rock has experienced since burial. It is not a thermochronometer *per se*, in that it does not provide an age or any other direct indication of time.

3.4.2. Deposition age and passive mode. Because the vitrinite system is initiated when sedimentary material with organic matter is deposited, HeFTy begins the vitrinite calculation as of the *deposition age* of the sample. The deposition age is defined for a given HeFTy time-temperature path as the time of minimum temperature that is not present-day and does not lie on a cooling-only path that ends at the present day. This temperature must also be below a limiting value of 25°C. If these conditions are met, the time-temperature history is said to contain a *deposition event*. If no deposition event is implied by the time-temperature path, then the entire path is used to calculate %Ro, but the result is given a greater-than sign (>) indicating that the %Ro value is at least as high as the number given, but may be higher because the peak temperature since deposition is unknown. Note that the deposition age in this case does not necessarily have anything to do with the stratigraphic age range on the Sample Information tab sheet. An illustration of this functionality is given in Chapter 4.

In *passive mode*, the part of the time-temperature history used to calculate %Ro is further restricted to the region that is constrained by the other thermochronometers in the model. For some research applications, investigators utilize AFT or (U-Th)/He to estimate the thermal maturity of sediments. In these cases, the desired information is the level of thermal maturity constrained by those systems, which corresponds to the earliest time in a sample's history that is reflected in the measured data. For fission-track analysis, this corresponds to the age of the oldest track estimated by HeFTy. For (U-Th)/He, this is taken as the time at which the grain retains approximately 1% of its final helium total. Note that even if a time-temperature path includes a deposition event as defined above, in passive mode if it is not constrained by another thermochronometer it will not be taken into account in the calculation.

3.4.3. The vitrinite input tab page. Figure 3-7 shows an example of the tab page for vitrinite reflectance. The fields are:

- *Calibration*. There is currently only one vitrinite reflectance calibration in HeFTy, the widely used EASY %Ro method of Sweeney and Burnham (1990). Additional calibrations may be entered if there is demand.
- *Measured value and uncertainty*. Measured data can be entered here if one of the objectives of the HeFTy analysis is matching these values. If these values are entered, closeness of match to the %Ro values will be taken into account when evaluating goodness of fit between model and measured data.
- *Passive mode*. Use this check box to activate or deactivate passive mode, as described in section 3.4.2.

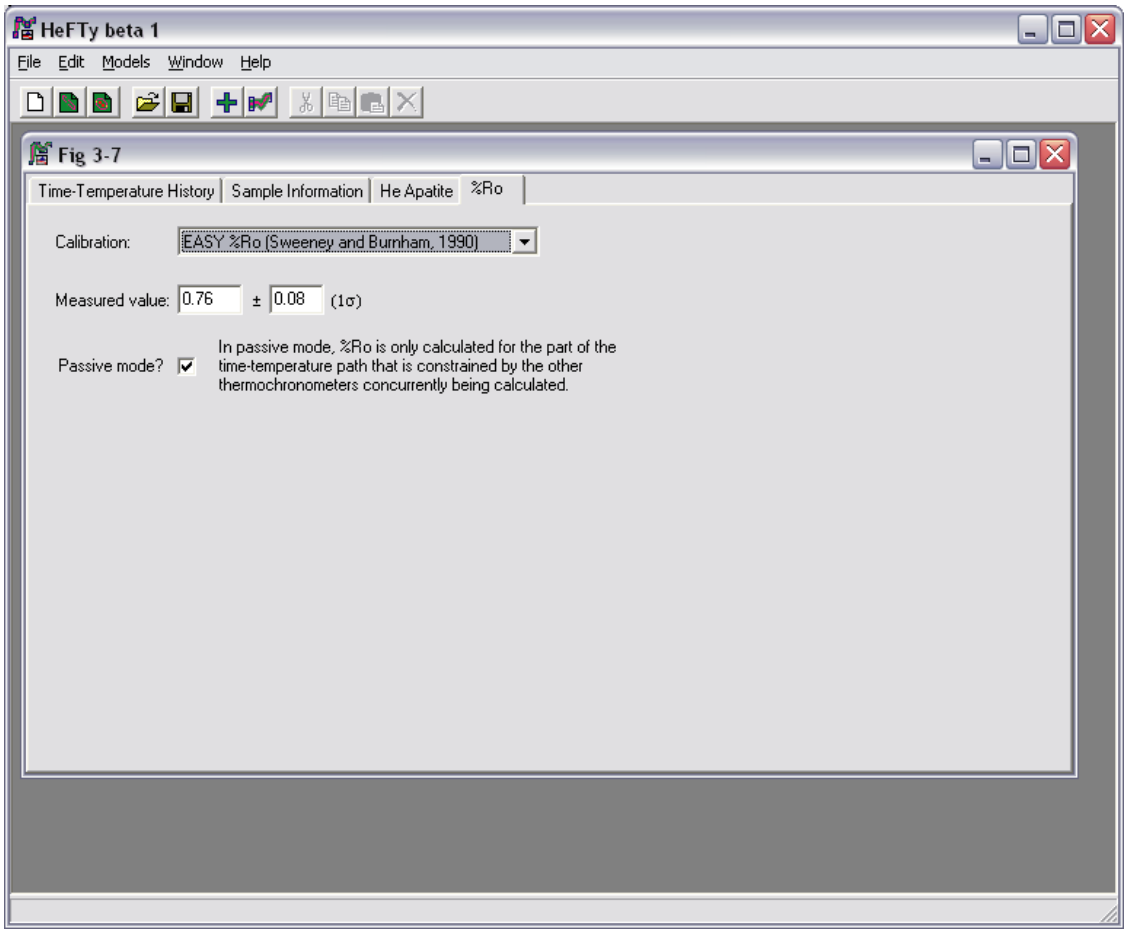

Figure 3-7. The vitrinite reflectance data and parameter entry tab page.

3.4.4. The vitrinite output panel. Figure 3-8 shows a pair of examples of the vitrinite output panel as it appears on the time-temperature history tab page. In the left frame, the time-temperature history includes a deposition event, so the model vitrinite result (0.44) is absolute, and its goodness-of-fit with the measured data is evaluated. In the right frame, the time-temperature history used for vitrinite calculation does not include a depositional event, so the result is given a ">" sign and GOF is assumed to be 1.00, indicating no quantifiable mismatch between model and data.

Figure 3-8. Example vitrinite reflectance output frames

4. Forward Modeling of Data

4.1. Introduction

The notion of forward modeling, as used here, is the process of predicting what thermochronometer measurements one would expect for a sample that has undergone a particular temperature history. By superimposing measured data, a comparison between the predicted results and measured values is possible. HeFTy does both of these things and also permits interactive modification of time-temperature histories and continuous updating of model predictions.

HeFTy can also be used in this mode to quickly and easily determine whether one or more thermochronometric systems will be useful for solving a particular geological problem. If the investigator has an idea of what the possible time-temperature histories are for a sample, those histories can be entered to see how different the expected fission-track and/or (U-Th)/He results would be for each one, and determine which systems or set of systems are most likely to differentiate between these histories. This information can be used to make more efficient use of resources when formulating a plan for investigation.

4.2. Model Statistics

4.2.1. Thermochronometer results. Figure 4-1 shows an example of an apatite fission-track data set fitted using HeFTy in a forward modeling sense. Here the data are split into two kinetic populations, using the division shown in Figure 4-2. Below the track length histograms are listed the following information for each kinetic population:

Model Age (Ma) is the fission-track age predicted by HeFTy.
Measured Age (Ma) is the pooled age from the measured data.
Age GOF is the goodness-of-fit between the model and measured ages (see below)
Oldest Track (Ma) is the age of the oldest fission track to survive annealing in the model simulation.
Model Length (μm) is the mean and standard deviation of the track length distribution predicted by HeFTy.
Measured Length (μm) is the mean and standard deviation of the measured track length distribution.

Length GOF is the value of the goodness-of-fit statistic (Kolmogorov-Smirnov test or Kuiper's statistic; see below) for comparing the model to the measured length distribution.

For (U-Th)/He thermochronometers, the results reported are the measured and models ages, and their GOF.

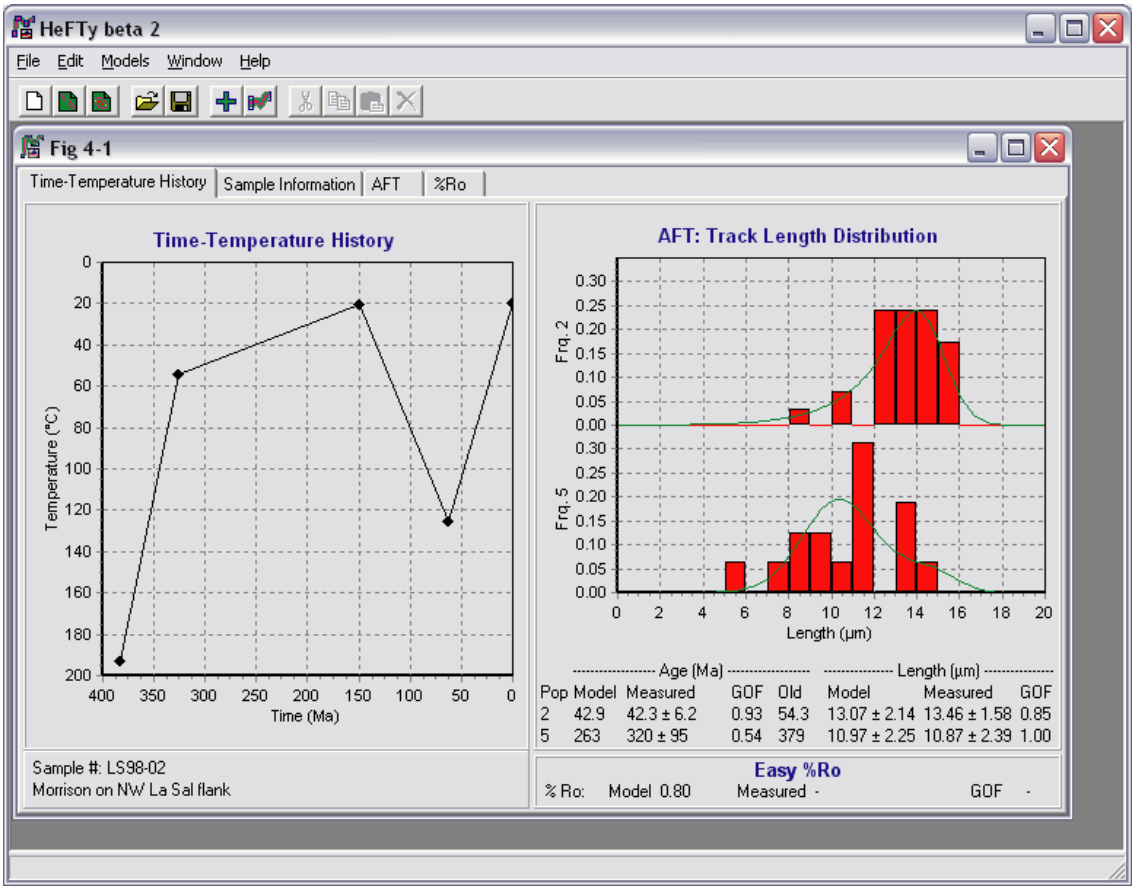

Figure 4-1: Example of a single forward model run of HeFTy that closely fits a set of measured apatite fission-track data. Peak burial is at 62.6 Ma and 125.4°C.

Two statistics are used to gauge how well the data and the model results match: one for the fission-track length distribution, and another for the age. This approach is described in detail in Ketcham et al. (2000) and Ketcham (2005). The two available methods for comparing the fission-track length distribution to the track length distribution predicted by the model are the Kolmogorov-Smirnov test (or K-S Test) and Kuiper's Statistic (see section 3.2.4.3.1). The "Age GOF" is the goodness-of-fit between the age data and age predicted by the model.

4.2.2. "Good" and "Acceptable" fits. For each of these statistics, a "good" result corresponds to a value of 0.50 or higher, which is the expected value if the time-

temperature path and kinetic model are in fact the correct ones. An "acceptable" result corresponds to a value of 0.05 or higher; these values indicate that the model has not failed the null hypothesis test that forms the basis of these statistics. A model is considered "good" if all statistics for all populations being modeled are above 0.50 (as in the case of the model in Figure 4-1); similarly, a model is considered "acceptable" if all statistics for all populations are above 0.05. A useful way to think of these relative degrees of fitting is that a good result implies the time-temperature path is *supported* by the data, while an acceptable time-temperature path is *not ruled out* by the data. In the example shown here, there is a good match between the model and data for both data types in both populations.

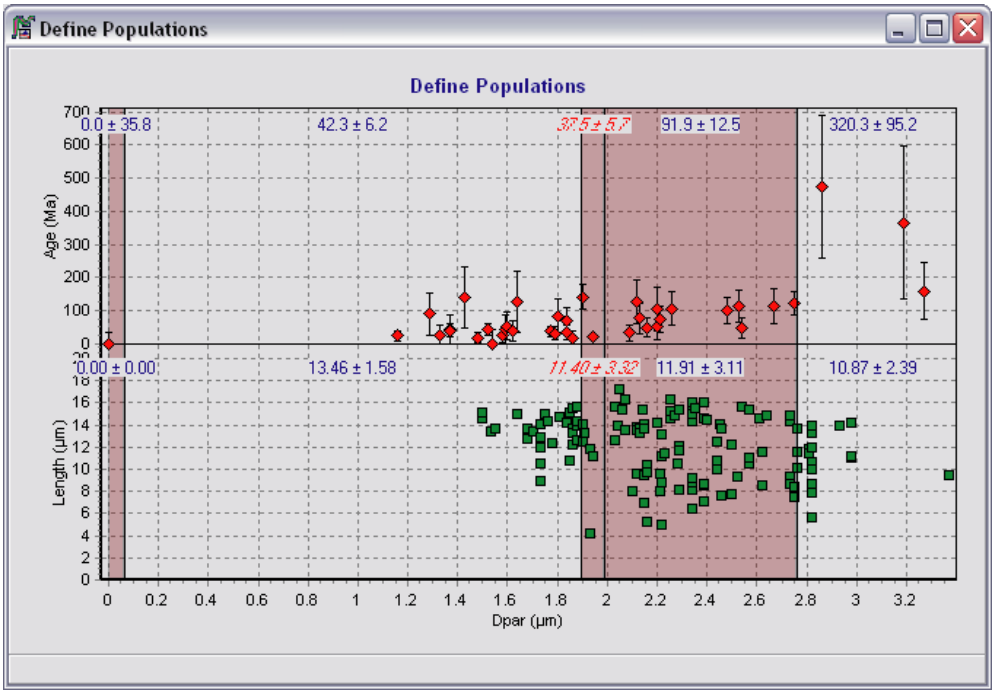

Figure 4-2: Kinetic populations modeled in Figure 4-1 (also see section 3.2.4.2). Shaded populations are omitted from mpdeling.

4.2.3. Predicted vitrinite reflectance. The model in Figure 4-1 also shows an equivalent vitrinite reflectance value. The Easy %Ro calculation for vitrinite maturation uses the method of Sweeney and Burnham (1990; see section 3.4 for details of the calculation in HeFTy). The method of calculation is dependent upon the time-temperature path currently being modeled, and on the kinetics of the current apatite system, and is mainly applicable to the modeling of sedimentary basins. Two possibilities are illustrated by the two kinetic populations in Figure 4-1:

1. For the lower-resistance population (population 2), the 57.3 Ma age of the oldest fission track to survive annealing (the error on this estimate probably ~6

Ma, proportional to the error on the measured age) is less than the 150 Ma stratigraphic age of the sample (this rock is a piece of Jurassic-aged Morrison formation from the flanks of the La Sal Mountains in Utah). For this sample, only the portion of the temperature history that occurred since 54.3 Ma can be used to calculate vitrinite reflectance equivalent; this calculated value serves only as a minimum. The Easy %Ro result is >0.64 (this is not shown in Figure 4-1 because of the presence of the high-resistance population; it can be seen if the higher-resistance population is temporarily removed from the calculation).

2. The higher-resistance population (population 5) has an oldest track of 379 Ma, greater than the 150 Ma stratigraphic age of the sample. For this population, the whole portion of the temperature history since 150 Ma is used to calculate vitrinite reflectance equivalent; this calculated value of 0.80 serves as an estimate of the actual maturity level.

4.3. Discussion

The model in Figure 4-1 offers several interesting insights. First, the degree of thermal maturity is fairly well determined by the 0.80 vitrinite reflectance equivalent calculated for the higher-resistance population. Also, the timing of peak burial temperature may be preserved in the data, as it appears to have occurred at least 57 Ma before present. This estimate of timing is consistent with known Laramide-aged cooling events throughout the western United States, including Utah.

Just how well constrained is this temperature history? Figures 4-3 through 4-6 attempt to illustrate this; the results of these models are summarized in Table 4.1. Acceptable models exhibit the following ranges in these parameters: (a) vitrinite reflectance equivalent, 0.64-1.19 with a preferred range defined by good models of 0.72-0.81, (b) peak burial temperature, 101.4-154.9°C with a preferred range of 114.1-126.8°C, and (c) timing of peak burial temperature, 43.7-81.1 Ma, with a preferred range of 52.7-65.5 Ma.

Table 4-1: Variation in (a) vitrinite reflectance equivalent value, (b) peak burial temperature, and (c) timing of peak burial temperature between forward models designed to explore the range of possibilities for the data modeled in Figure 4-1.

	Population 2		Population 5				
Figure Number	**Len. GOF**	**Age GOF**	**Len. GOF**	**Age GOF**	**Easy Ro (%)**	**Max. Temp. (°C)**	**Time of Max. Temp. (Ma)**
Fig. 4-1	0.85	0.93	1.00	0.54	0.80	125.4	62.6
Fig. 4-3	0.87	0.06	0.98	0.52	0.80	125.4	43.7
Fig. 4-4	0.80	0.06	1.00	0.57	0.80	125.4	81.1
Fig. 4-5	0.86	0.05	0.20	0.05	1.19	154.9	62.6
Fig. 4-6	0.78	0.05	0.54	0.82	0.64	101.4	62.6

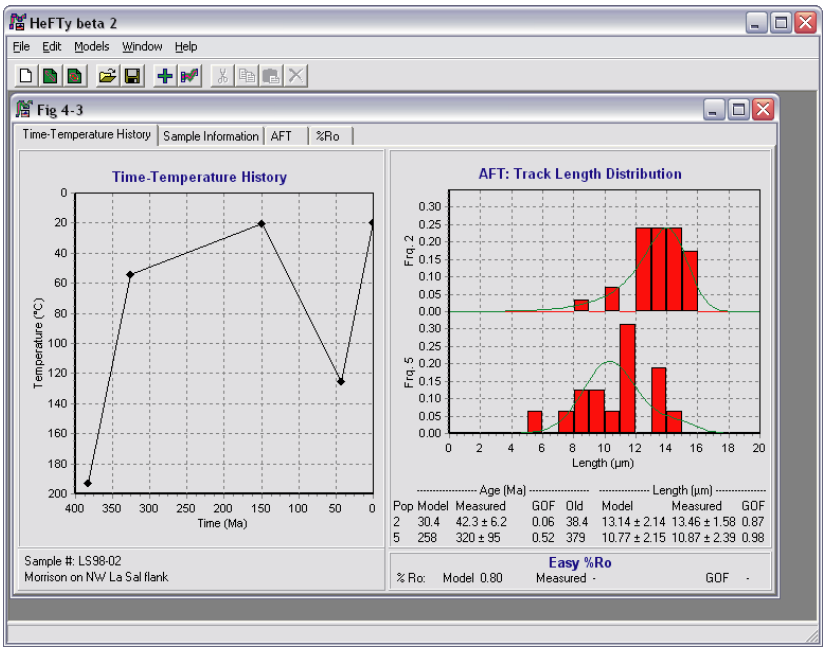

Figure 4-3: The same model as in Figure 4-1 except the time of peak burial temperature is shifted to 42.7 Ma. Note that the age GOF value for population 2 is barely acceptable, as it is the parameter that is most sensitive to this shift in timing of peak burial.

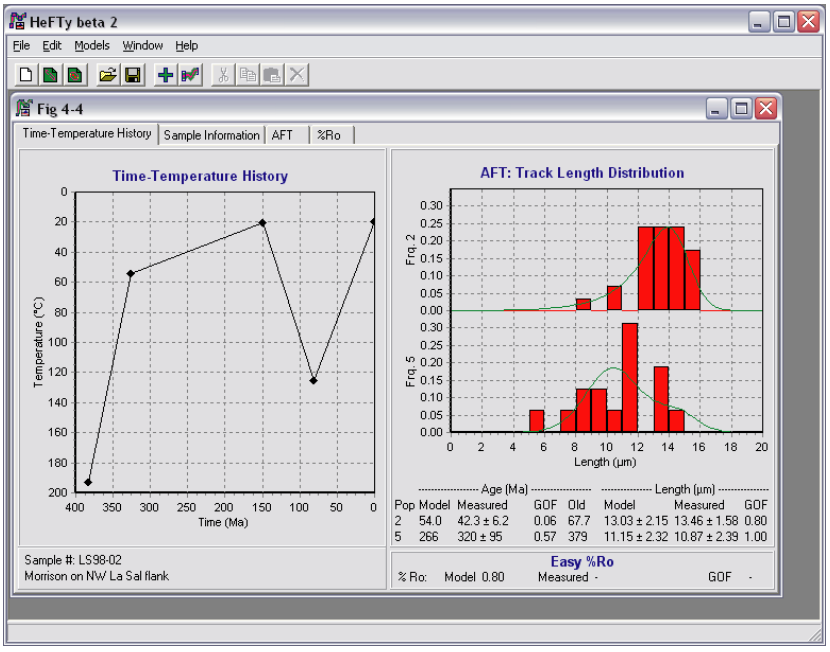

Figure 4-4: The same model as in Figure 4-1 except the time of peak burial temperature is shifted to 81.1 Ma. Note that the age GOF value for population 2 is barely acceptable, as it is the parameter that is most sensitive to this shift in timing of peak burial.

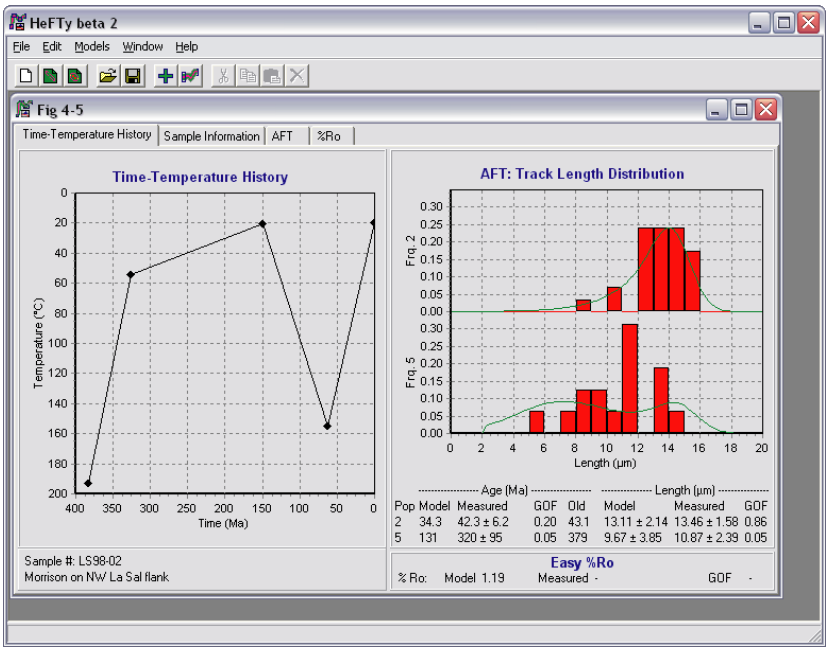

Figure 4-5: The same model as in Figure 4-1 except the peak burial temperature is shifted to 154.9°C. Note that three of four GOF parameters have fallen, and two are barely acceptable.

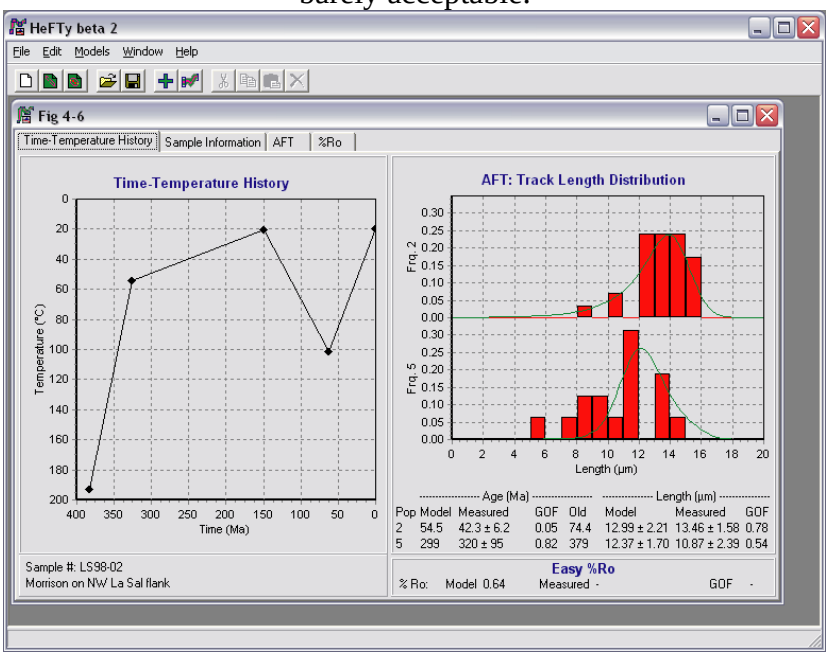

Figure 4-6: The same model as in Figure 4-1 where the peak burial temperature is shifted to 101.4°C. Note that statistical parameters for both populations have gone down.

5. Inverse Modeling of Data

5.1. Introduction

The notion of inverse modeling, as used here, is the process by which (a) a large number of forward models are generated by HeFTy, (b) the predicted thermochronometer results are compared to the measured values for each forward model, and (c) the good and acceptable forward models (defined in section 4.2) are used to provide quantitative constraints on time-temperature histories that are permitted by the measured data.

5.2. Running the Inverse Model

The following procedures must be performed to set up and execute the inverse model:

5.2.1. Preliminary steps. First, a new model file must be created, with the desired thermochronometers and their corresponding data added. The method for creating files and adding thermochronometers are given in Chapter 2, and procedures for loading data into each thermochronometer are described in Chapter 3. An example file ready for inversion is shown in Figure 5-1. This is the same setup as shown in Chapter 4, with an apatite (U-Th)/He thermochronometer added. Figure 5-1 also shows the result of a preliminary forward model; some forward modeling is often a useful step to establish that the data can be fitted and to help guide setup of the inversion.

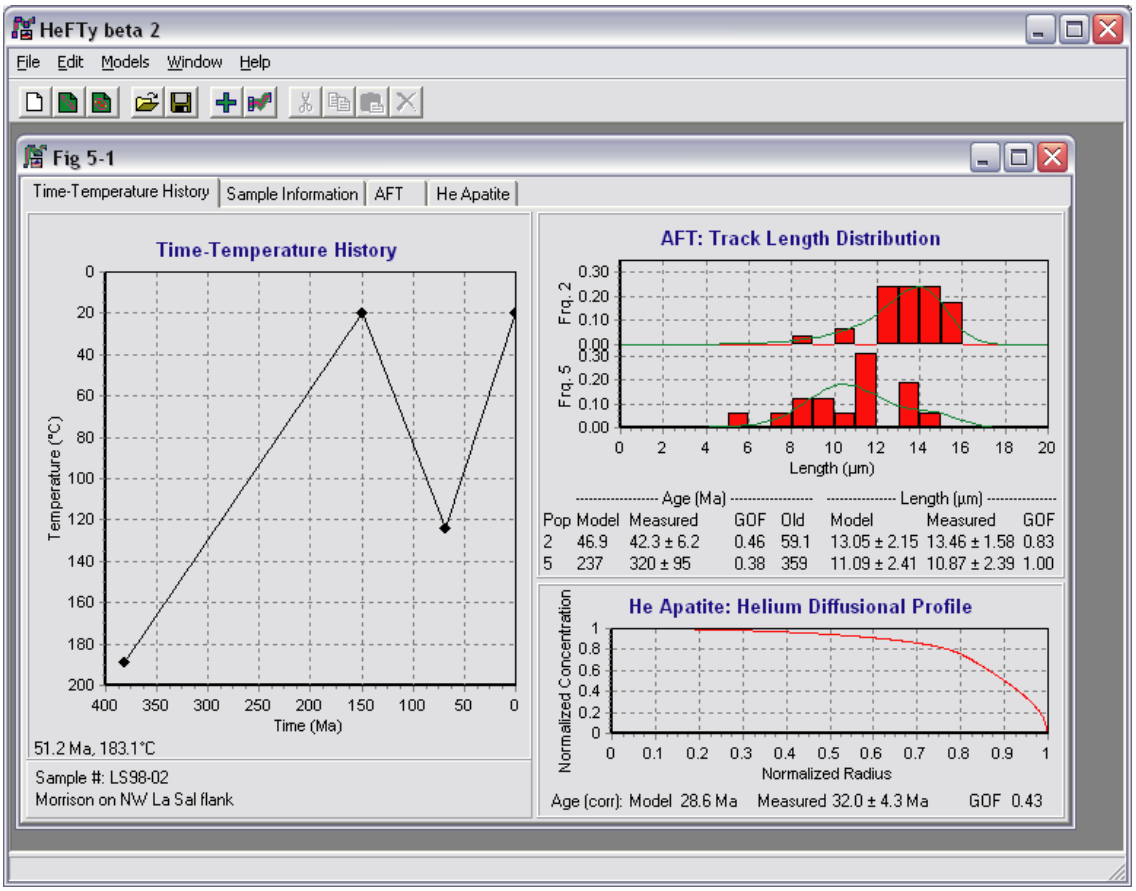

Figure 5-1: Model file ready for inversion. Two thermochronometers and their corresponding data have been added: one apatite fission-track and one (U-Th)/He. The AFT data have been divided into two kinetic populations, as shown in Chapter 4.

5.2.2. Entering Inverse Modeling mode. Next, press the "Inverse modeling" button, to the right of the "Add thermochronometer", or "+" button, to bring up the inverse modeling dialog (Fig. 5-2).

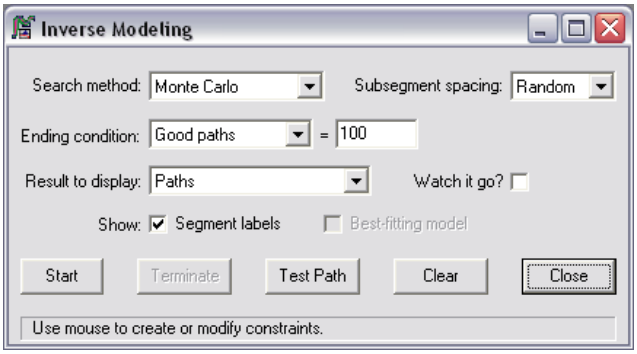

Figure 5-2: The *Inversion Modeling* dialog box.

5.2.3. Specifying constraints in the time-temperature window. In the main program window, the forward model time-temperature path has been grayed out. This indicates that it can now be used to define the constraints to be used for inverse modeling. Now, clicking and dragging the mouse in the time-temperature window will create a series of boxes, through which the time-temperature histories will be forced to pass. These boxes are called *constraints*, and the path of the time-temperature path connecting two constraints is called a *segment*. One constraint is always automatically defined at the time=0 axis (i.e. the present day). Figure 5-3 shows the main program window after the first new constraint has been created.

The constraints consist of a series of blue boxes, with their center points connected by labeled orange lines. Constraint boxes can be resized by clicking and dragging their corner points. They can be deleted by right-clicking on their center points to bring up a pop-up menu, and choosing the "Delete Constraint" option.

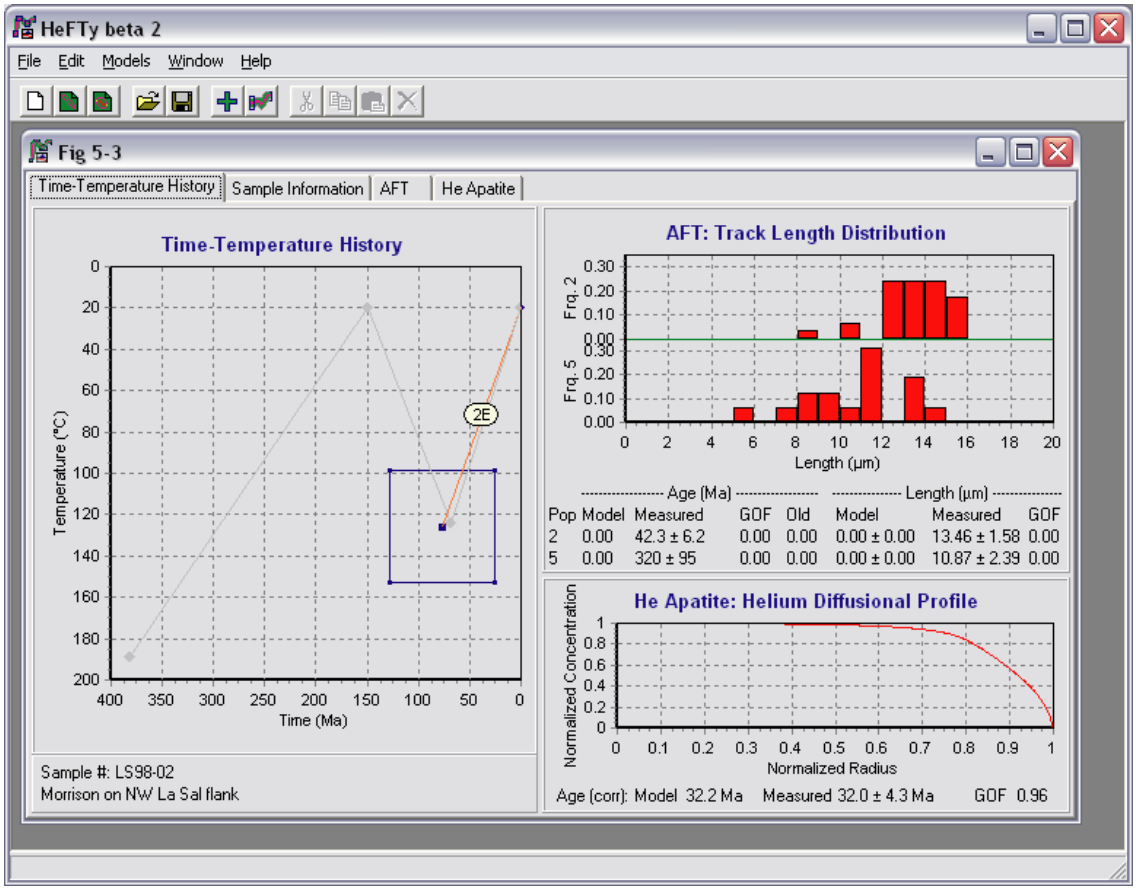

Figure 5-3: File window after creation of first inverse model constraint (blue box). Paths generated for inverse modeling are forced to go through all boxes specified.

Constraints can overlap each other to a considerable degree. The only limitation is that, if a one constraint begins before another (i.e. has an earlier starting time), it must also end before it (have an earlier ending time). The software automatically enforces this limitation when constraints are entered.

5.2.4. Segment codes. The "2E" code on the line between the two constraints in Figure 5-3 denotes how HeFTy will interpolate the time-temperature path on the segment between those two constraints. The code has the format *nT*(/*r*), where:

- *n* is the number of times the segment between constraints is halved by introducing new nodal points allowing a change of slope. During time-temperature path generation, 2^{n-1}-1 nodal points are interpolated along the path between constraints, breaking the segment into 2^n sub-segments.
- *T* is the type-code for the randomizer that generates the interpolating node points and path segments. The codes are
    - E (episodic), in which the path is subject to sudden changes. This mode may correspond to unroofing dominated by periodic movement of normal faults.
    - I (intermediate) in which the path is less prone to sudden changes, but may experience them occasionally. This may correspond to burial by periods of fast sedimentation punctuated by quiescent intervals, similar to what is often implied by basin subsidence modeling.
    - G (gradual), in which changes are mostly gradual, as may be expected for consistent burial or slow, erosion-dominated unroofing.
- *r* is an optional maximum heating or cooling rate (in units °C/Myr) that is imposed on each subsegment between the two constraints. If this option is used, the heating rate or cooling rate will never go above the value chosen. Note that this option can interact with the randomizer mode chosen, in that an "episodic" section of the path may be forced to be gradual if a low maximum heating/cooling rate is imposed.

5.2.5. Changing segment properties. The settings for any segment can be changed by double-clicking on its label, or right-clicking on it and choosing the "Edit Segment Parameters…" option, opening the dialog in Figure 5-4. This dialog allows all of the parameters mentioned in section 5.2.4 to be set, plus one more. Paths between constraints are always monotonic (cooling-only or heating-only). However, if the temperature ranges of consecutive constraints overlap, those constraints can be connected by either heating or cooling paths. The "Path between constraints" option allows these situations to either be "Monotonic Consistent", meaning that they will always have only one direction (depending on the relative temperatures of their center points), or simply "Monotonic", meaning that both types of paths may be generated.

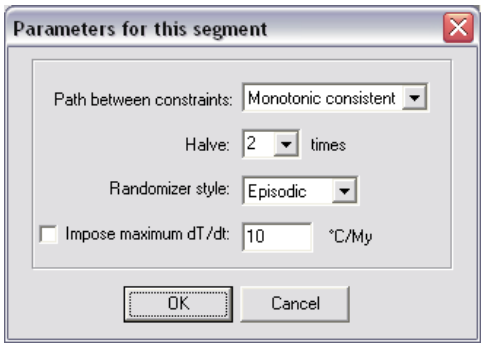

Figure 5-4. Dialog for editing segment parameters.

5.2.6. Ending conditions. The Inverse Modeling dialog box (Fig. 5-2) provides three options for specifying how an inversion is to be completed. The are:

- *Paths tries = n*. Creates and evaluates n independent time-temperature paths.
- *Good paths = n*. Continues creating and evaluating paths until *n* paths pass the "good" criterion (see section 4.2).
- *Acceptable paths = n*. Continues creating and devaluating paths until *n* paths pass the "acceptable" criterion (see section 4.2).

5.2.7. Subsegment spacing. This option in the Inverse Modeling dialog box (Fig. 5-2) controls whether subsegments are created at even or random time intervals; i.e. whether the each subsegment connecting two constraints will have the same duration or not. The main purpose of this option is to allow older AFTSolve-style models (even-interval) to be generated for instructional or comparative purposes; it is recommended that the "Random" option always be used in standard practice.

5.2.8. "Watch it go" option. If this box is checked, each time-temperature path generated and evaluated is shown on the computer screen as the inversion progresses. This option can be used to give the operator a sense of the forms of the paths being generated, or to reassure the operator that HeFTy is functioning properly. However, this function should be turned off most of the time, as it consumes significant computer resources, causing inversions to take significantly longer to complete.

5.2.9. "Test Path" button. Once all constraints have been added and their segment parameters and other controls set, this option can be used to generate a path that meets the criteria specified, allowing the operator to verify that the path generator will behave as expected. Figure 5-5 a test path connecting the series of constraints that will be used for the example inversion in this chapter.

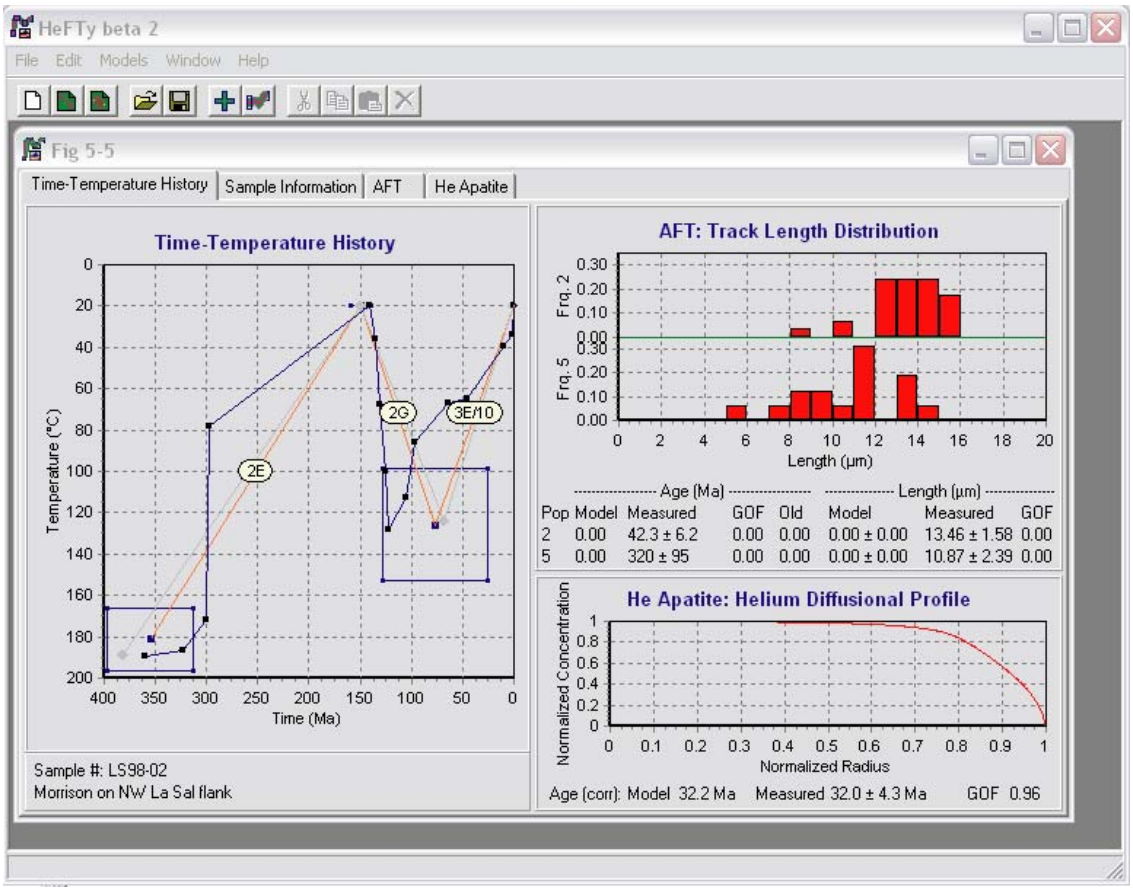

Figure 5-5. Model with all constraints and parameters entered, and a test path.

5.2.10. Start/Pause and Terminate buttons. These controls allow the inversion process to be started and stopped. The "Start" button starts the inversion. When an inversion is underway, this button changes to "Pause", which can be used to temporarily suspend inversion, with restarting allowed. The "Terminate" button stops the inversion process entirely; it is only enabled when the inversion is underway.

While an inversion is running, most of the HeFTy user interface is turned off; the only controls the user can access are Watch it go (5.2.8), Results to display (5.2.11) and Pause and Terminate. However, during inversion the user may work in other programs while HeFTy toils in the background.

During inversion, the lower part of the Inverse Modeling dialog continually updates inversion progress by reporting the number of paths tried and the number found that meet the necessary criteria, and estimates the time remaining until completion. When an inversion ends, either by running to completion or being terminated, the dialog displays the final results.

5.2.11. Results to display. HeFTy has three ways of displaying inversion results:

- *Paths*. Each good path is displayed as a magenta line, and each acceptable path is displayed as a green line. This mode is recommended for viewing results as they accumulate during inversion.
- *Path envelopes*. The region encompassing all good paths is colored in magenta, and the region encompassing all acceptable paths is colored in green. It should be noted that not all possible paths that lie within these envelopes are expected to pass the criterion indicated by the envelope.
- *Constraint points*. Plot only the nodal points that lie inside constraint boxes; good points are magenta, acceptable are green. Because most constraints represent local temperature maxima or minima, this option is good to examining the times and temperatures of peak heating found by the inversion procedure.

This option can be changed after an inversion is completed. It is best to keep it on the "Paths" setting during the inversion process, as the inversion envelopes are not calculated until after the inversion has been completed. Figure 5-6 shows a completed inversion model run using the starting conditions shown in Figure 5-5, with examples of all three display modes.

5.2.12. Clear button. This button clears all results from a completed or terminated inversion. Clearing is required for changing some of the inversion parameters, so as to avoid the appearance

5.2.13. Show segment labels and best-fitting model options. These buttons respectively control whether HeFTy displays the segment labels discussed in section 5.2.11, and the time-temperature path for the best-fitting model in a completed inversion.

5.2.14. Close button. This button closes the Inverse Modeling dialog box, and puts HeFTy back into forward modeling mode. All aspects of the inverse model (constraints, segment labels, inversion results) are erased from the screen; however, they can be brought back by opening the Inverse Modeling dialog box again. Inversion results are saved when the file is saved.

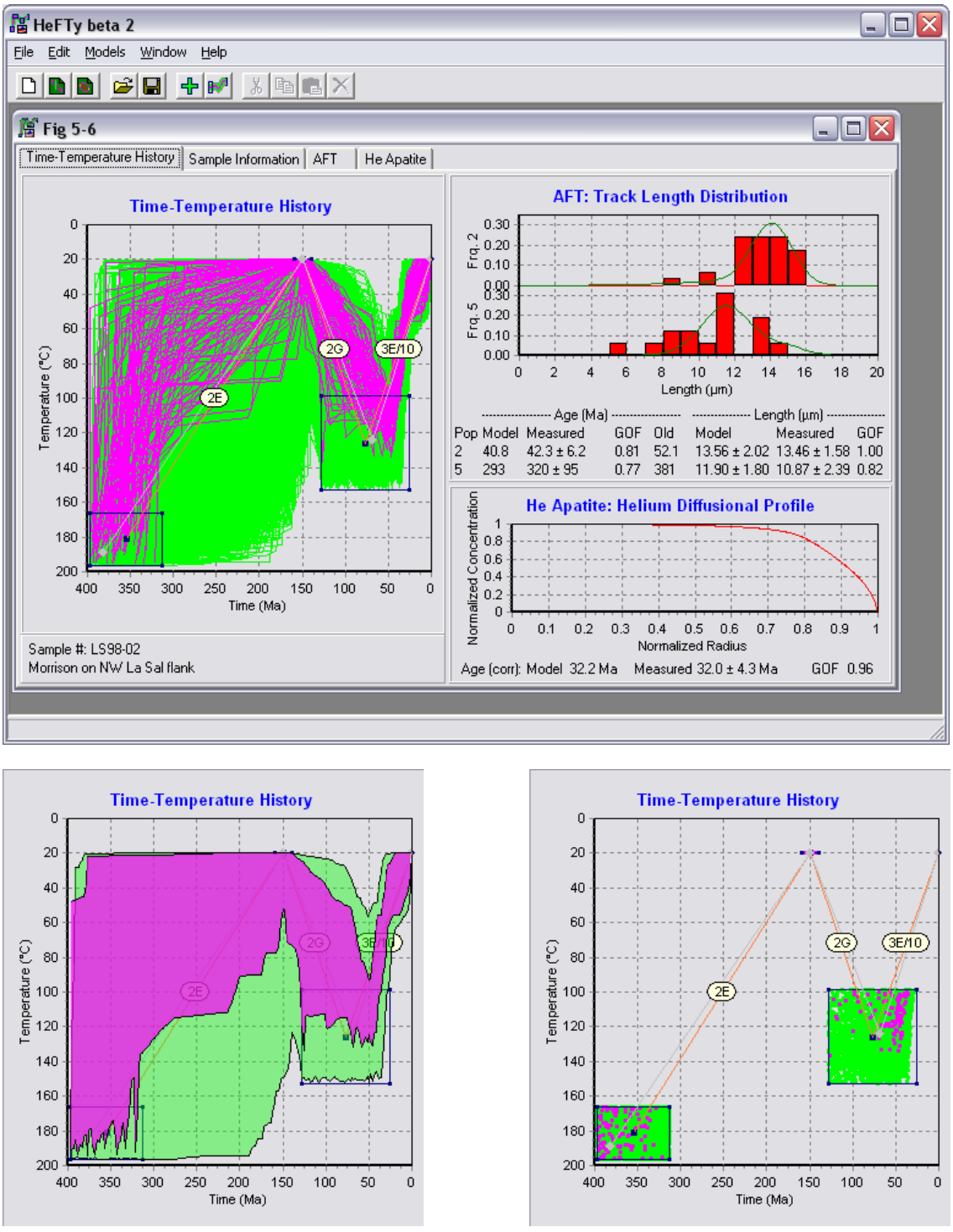

Figure 5-6. Completed inversion model. Upper window shows "Paths" result display and the result for the model that best fits all AFT and AHe data. Lower left shows "Path Envelopes" result display, and lower right shows "Constraint Points" result display.

5.3. Discussion

Inverse models have the distinct advantage over forward modeling by hand of permitting many thousands of forward models to be calculated for a sample, subject to whatever constraints the user can bring to bear on the time-temperature history. As such, it is common to obtain hundreds or even thousands of acceptable time-temperature histories. With so many solutions, it is often possible to obtain an interpretation that is sensible and tightly constrained. Indeed, determining the degree to which a thermal history is constrained by thermochronometric data is often the goal of inverse modeling.

However, although it is tempting to think of inverse modeling as objective, driven by ingenious algorithms and iron-clad statistics, it is closer to the truth to say that using inverse modeling software such as HeFTy is part art and part science. In particular, it must be understood that the way a user sets up an inversion can have almost as much influence on the results as the data themselves.

One of the philosophical issues underlying inversion schemes is how "complex" the actual time-temperature history experience by any particular rock body in the Earth is. Does its temperature evolve smoothly and slowly over millions of years due to the nature of the crust as a low-conductivity thermal boundary layer? Or could it be jagged or even chaotic, subject to sudden, albeit minor, excursions due to more temporally variable processes such as fluid flow, intrusive activity, tectonic unroofing, and conductive propagation from climate changes at the Earth's surface?

Part of the design of HeFTy is to put the ability to make this choice and study its ramifications into the geologist's hands. The amount of complexity allowed is explicitly controllable by manipulating the number of interpolated nodes, the randomizer style, and the maximum allowable heating and cooling rates. In general, fewer nodes and more tightly limited rates will lead to fewer good and acceptable paths, and the appearance of a more well-bounded range of possibilities. Conversely, increasing the allowed complexity can greatly expand the range of solutions, but will also increase one's level of confidence that the results more fully represent the full range of possibilities allowed by the data, rather than artificially bounded by limitations implicitly imposed by the model and modeler.

The inversion results shown in Figure 5-6 illustrate this point. The model allows quite complex paths, and as a result a wide range of time-temperature histories fit the data well. Consequently, the timing of the post-depositional thermal peak is not firmly bounded, and the data can be well-fitted by any possibility from 36 to 130 Ma. However, there is a strong cluster of peaks among the good fits from 55 to 45 Ma, corresponding to a Laramide event as would be expected for this locality. The data thus do not require a Laramide event, but are supportive of it.

The best use of inverse modeling will in part depend on the geological situation, the geological problem being solved, and the thermochronologic data themselves. Given the range of objectives and circumstances, there are probably a number of ways of doing inverse modeling "right."

Further discussion of the various inverse modeling options and strategies can be found in Ketcham et al. (2000) and Ketcham (2005b).

6. Additional Functions

6.1. Introduction

This chapter covers various additional aspects of HeFTy functionality not discussed elsewhere, such as batch modeling, time-temperature path importing, and setting program preferences.

6.2. Batch Modeling

Inverse models can also be run in batch mode, in which HeFTy reads a list of files and specifications and runs a series of inverse models. This can be very useful for running large numbers of fits; HeFTy can be left to run overnight on most computers, completing tens of inverse models.

The first stage of setting up a batch model is to create a file and enter the thermochronometric data to be fitted. Then, two approaches can be used:

1. Enter all f the fitting parameters through the program interface, reproducing all steps described in section 5.2 except pressing the "Start" button. Then, save the file, and create a "Type 1" batch file, as described in Appendix C.1.
2. Save the file as-is, and use a "Type 2" batch file (as described in Appendix C.2) to specify the inversion parameters.

Once a batch file has been properly set up, it can be executed using the "Run Batch File…" option under the "Models" menu. Choosing the menu option will call up a dialog asking for the location of the batch specification file. Once the file is selected, the batch run begins immediately. If any inversion during a batch run is terminated, the entire batch run is terminated. However, inversion during batch runs can be safely paused and restarted.

6.3. Importing Time-Temperature Paths

The "Import time-temperature path…" option in the "Models" menu allows a time-temperature path to be read in from a text file (format described in Appendix A). This can be used to perform calculations based on thermal histories calculated in other programs. This option can also be used to circumvent the limitation in the user interface of the minimum temperature being 0°C.

6.4. Preferences

6.4.1. Introduction. The "Preferences…" option in the "File" menu brings up a dialog that allows the user to control many aspects of HeFTy's behavior, including default values for thermochronometers parameters and conversion factors for data import. The Preferences dialog uses a tab-page format, with one page for general settings and others for thermochronometers.

6.4.2. The General Preferences tab page. Figure 6-1 shows an example of this tab page. The only preferences that are set here are the default maximum values for the time and temperature axes on the time-temperature history graph..

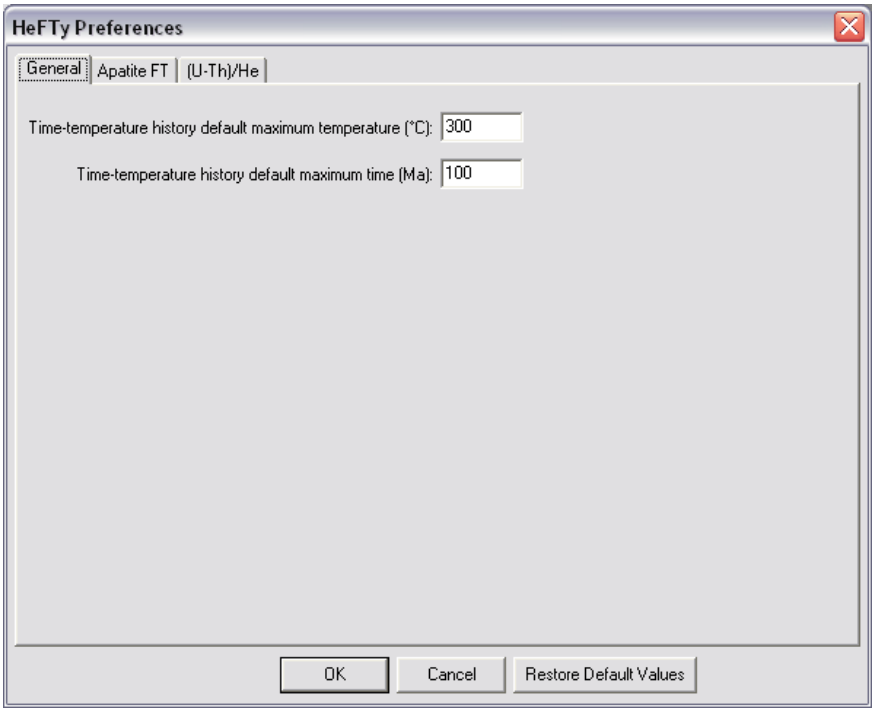

Figure 6-1. The General Preferences tab page.

6.4.3. The Apatite FT Preferences tab page. This tab page (Fig. 6-2) is divided into three sections. The upper section allows default values to be set for many of the calibration settings and parameters on the AFT input tab page (section 3.2.4). The middle section allows the user to customize how initial track lengths are estimated when length data are imported into the program (section 3.2.4.3). The bottom section is for D_{par} conversion factors, permitting users to make their measurements compatible with the Carlson et al. (1999) data set and Ketcham et al. (1999) annealing model, and for setting default values for the horizontal axes in the "Define Populations" dialog (Fig. 3-2).

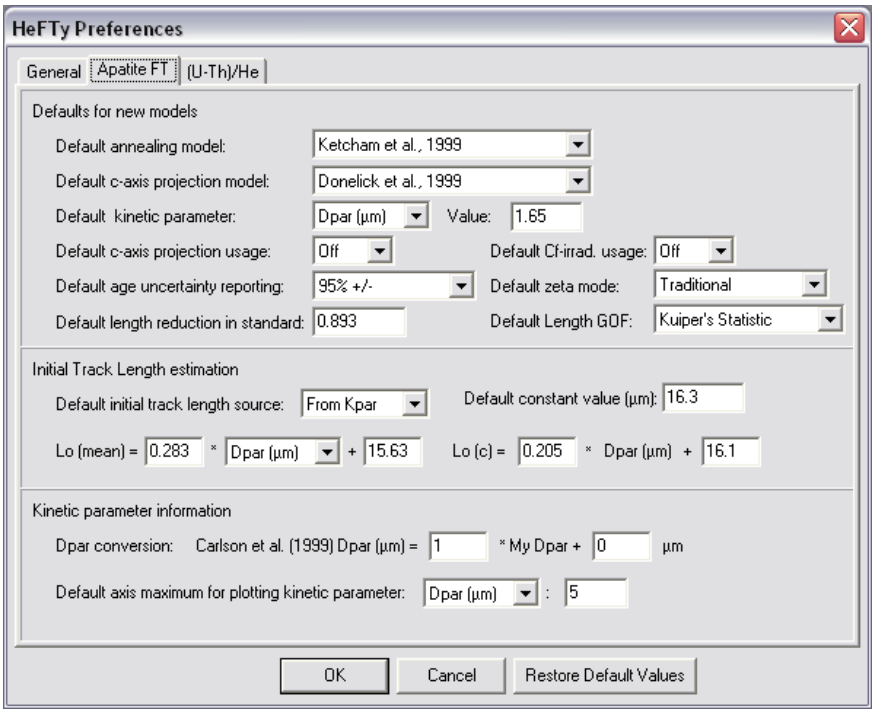

Figure 6-2. The Apatite FT Preferences tab page.

The initial track length estimation section allows the user to either specify a constant value that is always used, or a set of linear conversion from any of the defined kinetic parameters to initial mean length and initial mean *c*-axis-projected length. The bottom line of this section allows the entry of the linear conversion factors for any kinetic parameter; when a kinetic parameter is chosen from the drop-down list, the associated conversion factors are displayed in the text fields, where they can be edited. The default values are from Carlson et al. (1999).

The top line of the bottom section allows entry of a linear conversion between the D_{par} values reported by Carlson et al. (1999) and values measured by the analyst whose data are being analyzed. Conversion factors can be derived by measuring etch figures in some of the apatites studied by Carlson et al. (1999). Note that this conversion takes place "behind the scenes": the D_{par} values as seen in the program interface will be unaffected, but when used to estimate kinetic behavior they will be revised by this function. However, they will not be converted for initial track length estimation; it is assumed that the conversion function entered in the middle section of this page uses D_{par} values s measured by the analyst. *[An alternative to using this function is to convert the Dpar values before they are imported into HeFTy]*.

6.4.4. The (U-Th)/He Preferences tab page. This page is divided into two sections (Fig. 6-3). The upper section is for entry of default values for various parameters in the (U-Th)/He input tab page (section 3.3.4). The lower section allows the user to enter parameters for a diffusion calibration not preset in HeFTy. Whenever the user selects the "Other" calibration option in the (U-Th)/He input tab page, the

parameters here will appear as a default, although they can be changed freely. Changes to these parameters in a (U-Th)/He input tab page will not affect the Preference settings. *[Users can send notifications of new calibrations to the program author for incorporation into future versions]*.

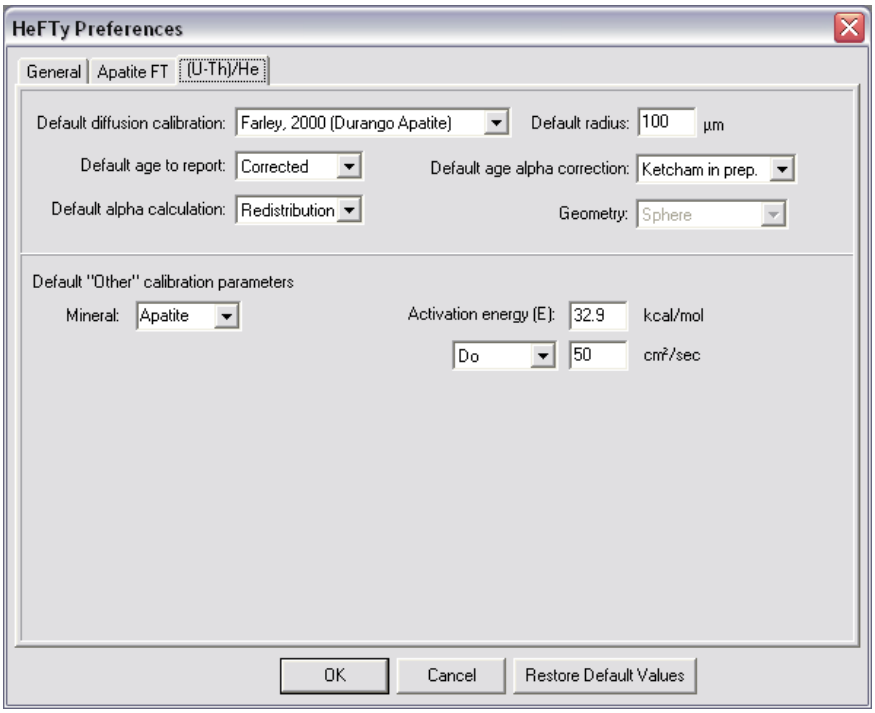

Figure 6-3. The (U-Th)/He Preferences tab page

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Appendix A: Example Input Data Files

A.1. Introduction

Many types of data can be entered into HeFTy using tab-delimited text files. Examples of these files accompany the HeFTy distribution, and are compiled into the Microsoft Excel spreadsheet “Import Templates.xls”.

Most of the input files allow up to 20 header lines, which can be anything, after which there is a "keyword" line defined by starting with a certain key word. For example, in the FT age files, the header is over when a line begins with the word "Zeta." After this point the file must adhere strictly to the format shown in the example data in each template.

A.2. Fission-Track Age Data File, Traditional Zeta

The “Traditional Zeta” age method follows the recommendation of Hurford and Green (1983). This file format begins with up to 20 header lines, with the header ending when a line begins with the word “Zeta:”. On that line, in the second column (i.e. after the first tab character, ASCII code 9), the word “Traditional” is used to indicate that the traditional zeta mode is being used. Next comes a line with four headers, separated by tab characters: “zeta” (zeta value), “sig zeta” (standard error of zeta), “rho-d (N/cm²)” (dosimeter density), and “Nd” (number of track counted for dosimeter). On the next line, again separated by tabs, are the values for these four parameters. The next line has three headers, separated by tabs: “Ns”, “Ni”, and the kinetic parameter type. Valid kinetic parameters headers are: “Dpar”, “Cl(wt%)”, “Cl(apfu)”, “OH(apfu)”, and “rmr0”. If no kinetic data are available, use one of the Cl headers, and use zeros for the corresponding data. Following this is a series of lines with these three values, one line per measured grain.

```
Sample Name
more info
whatever, up to 20 lines
Zeta: Traditional
zeta      sig zeta    rho-d (N/cm²)     Nd
118.9     3.6         3.6190E+06        4098
Ns        Ni          Dpar
```

```
6       8       3.27
21      36      2.75
4       8       2.2
7       13      2.67
.
.
.
```

A.3. Fission-Track Age File, Phi-Method Zeta

The "Phi-Method Zeta" age method follows the approach of Jonckheere (2003), which does not require an age calibration standard. This file format begins with up to 20 header lines, with the header ending when a line begins with the word "Zeta:". On that line, in the second columns (i.e. after the first tab character, ASCII code 9), the word "Phi(J2003)" is used to indicate that phi-method zeta mode is being used. Next comes a line with four headers, separated by tab characters: "zeta" (zeta value), "sig zeta" (standard error of zeta), "phi (n/cm²)" (neutron fluence), and "sig phi" (standard error of the same). On the next line, again separated by tabs, are the values for these four parameters. The next line has three headers, separated by tabs: "Ns", "Ni", and the kinetic parameter type. Valid kinetic parameters headers are: "Dpar", "Cl(wt%)", "Cl(apfu)", "OH(apfu)", and "rmr0". If no kinetic data are available, use one of the Cl headers, and use zeros for the corresponding data. Following this is a series of lines with these three values, one line per measured grain. Further details of the implementation of the phi method are in section 3.2.4.4.1 and appendix D.2.

```
Sample Name
more info
whatever, up to 20 lines
Zeta: Phi(J2003)
zeta     sig zeta   phi (n/cm²)    sig phi
0.55     0.014      2.35E+15       5.00E+13
Ns       Ni         Dpar
1002     2029       1.5
1351     2819       2
1073     1931       2.5
1087     1967       3
.
.
.
```

A.4. Fission-Track Age File, LAICPMS Ratio Zeta

The "LAICPMS Ratio Zeta" age method follows the approach of Donelick et al. (in review), which uses laser ablation inductively couples plasma mass spectrometry to measure U content in grains, rather than the external detector method. This file format begins with up to 20 header lines, with the header ending when a line begins with the word "Zeta:". On that line, in the second columns (i.e. after the first tab character, ASCII code 9), the code "LAICPMS ratio" is used to indicate the zeta mode. Next comes a line

with two headers, separated by tab characters: “zeta” (zeta value), and “sig zeta” (standard error of zeta). On the next line, again separated by tabs, are the values for these two parameters. The next line has five headers, separated by tabs: “Ns” (number of spontaneous tracks), “Area (cm²)” (area over which spontaneous track counted), “Pcorr” (corrected ratio between measured isotopes, for example (^{238}U /^{43}Ca), “sig(Pcorr)” (standard error of the same) and the kinetic parameter type. Valid kinetic parameters headers are: “Dpar”, “Cl(wt%)”, “Cl(apfu)”, “OH(apfu)”, and “rmr0”. If no kinetic data are available, use one of the Cl headers, and use zeros for the corresponding data. Following this is a series of lines with these three values, one line per measured grain.

```
Sample Name
more info
whatever, up to 20 lines
Zeta: LAICPMS ratio
zeta     sig zeta
13.07    0.014
Ns       Area (cm²) Pcorr      sig(Pcorr)  Dpar
10       0.000064   2.96E-02   5.66E-04    1.7325
6        0.000064   2.94E-02   1.14E-03    1.785
4        0.000064   3.06E-02   1.37E-03    1.84
4        0.000064   3.02E-02   1.46E-03    1.7967
9        0.0000576  3.14E-02   5.78E-04    1.8425
.
.
.
```

A.5. Fission-Track Length Data File

The fission-track length file format begins with up to 20 header lines, with the header ending when a line begins with the word “length”. On that line, there must be either three or four headers, separated by tab characters (ASCII code 9). The first two are “length” (track length in micrometers) and “angle” (track angle to c axis in degrees), and the last one is for the kinetic parameter. Valid kinetic parameters headers are: “Dpar”, “Cl(wt%)”, “Cl(apfu)”, “OH(apfu)”, and “rmr0”. If no kinetic data are available, use one of the Cl headers, and use zeros for the corresponding data. An optional fourth parameter, which should be in the third position if present, is “Lo” (initial track length). The Lo can optionally be followed by parentheses by the name of the kinetic variable that was used to estimate it. Following this is a series of lines with these three or four values, one line per measured grain. An example of a file with Lo:

```
Sample Name
more info
whatever
length   angle      Lo(Dpar)   Dpar
5        85         16.26      2.22
11.22    14.24      16.26      2.22
8.77     23.20      16.26      2.22
13.11    85.69      16.26      1.87
.
.
.
```

An example of a file without Lo:

```
Sample Name
more info
whatever
length   angle     Dpar
5        85        2.22
11.22    14.24     2.22
8.77     23.20     2.22
13.11    85.69     1.87
.
.
.
```

A.6. U-Th Zoing for (U-Th)/He

The file format for U and Th zoning begins with up to 20 header lines, with the header ending when a line begins with the word “Depth”. On that line, there must be three, separated by tab characters (ASCII code 9): “Depth” (distance below crystal surface, in µm), “232Thppm” (Th content) and “328Uppm” (U content). The depth is assumed to have its maximum value at the grain core, and a value of 0 at the rim. Following the header is a series of lines with these three values, one line depth:

```
Sample Name
more info
whatever, up to 20 lines
Depth (um)  232Thppm    238Uppm
66.663      2285.941    8588.826
66.598      2250.502    8739.653
66.531      2200.334    8719.302
66.476      2152.694    8550.183
.
.
.
0.103       495.927     272.546
0.036       504.11      273.344
0           501.819     270.87
```

A.7. Time-Temperature Path File

A time-temperature path input data file consists of 2 columns, separated by tabs. The first column is the time (m.y.b.p.; million years before present), and the second is temperature (°C). There is one line per time-temperature pair. The file should go from older to younger, with the oldest point as the first entry and the present-day point (i.e. zero age) as the lost entry. Points do not have to be evenly spaced in time. The data file can be any length; thousands or tens of thousands of time-temperature points can be provided, perhaps representing every time step in a thermal model. However, if there are more points that AFTSolve allows for user-entered forward models (50), then AFTSolve determines the best way to cut down the number of points to lose the minimum amount of

path information, and then informs the user of the largest amount of temperature error caused by the simplification. In general, errors will be a fraction of a degree C at most.

```
100.0     250.0
72.3      106.8
52.5      77.3
43.8      78.9
33.2      30.0
31.2      93.8
0.0       20.0
```

Appendix B: Output Data Files

B.1. HFT Format Files

Unlike AFTSolve, in which the "FMD" data files were readable in a word processor, HeFTy uses a binary file format that is only easily interpretable by HeFTy itself. HeFTy files can also grow quite a bit larger than AFTSolve files, as they retain all individual paths that fit the data during inversion.

Appendix C: Batch File Specification

C.1. Introduction

Batch files are tab-delimited text files, probably best created in a spreadsheet (e.g., Microsoft Excel), although a word processor or text editor can also be used. There are two types of batch files. Type 1 batch files are simply lists of HFT file names; for each name in the list, the file is opened, and the inverse model is run using whatever parameters are already entered into it, and the result is saved. Type 2 batch files allow specification of the inversion parameters.

The first line of any batch file begins with the title "BatchType:", followed by a tab and then the type number of the file.

C.2. Type 1 Batch Files: File names only

Batch files of the type containing file names only are ASCII text files created with a word processor or editor. An example batch file follows in which two inverse models are run using two individual HFT files. Each HFT file is overwritten by HeFTy upon completion of its respective inverse model:

```
BatchType:  1
c:/lasal1.hft
c:/lasal2.hft
```

C.3. Type 2 Batch Files: File names and fitting specs

After the header line specifying the batch file type, the sequence of lines for each model is as follows:

line 1: **input HFT file name**, with full directory path.

line 2: **output HFT file name**, with full directory path. If it is the same as the input file, the input file will be overwritten.

line 3: **title**. This replaces the title in the HFT file; enter a blank line if no change is desired..

line 4: **strat definition**. The first number is 0 if there are no stratigraphic age data, 1 if there is a single age, or 2 if the stratigraphic age is bounded by two values. This number is followed by the appropriate number of values, in Ma; if there are two values, start with the higher number.

line 5: **inversion specs**, corresponding to the input in the inverse modeling dialog. These are: modeling scheme (integer; Monte Carlo=0); ending condition type (integer; Paths tried=0, Good paths=1, Acceptable paths=2); number of paths (integer).

line 6: **number of time-temperature constraints** (integer).

subsequent lines: one line for each time-temperature constraint. Go from oldest constraint to youngest: first column = start time (Ma); second column = end time (Ma), third column = high temperature (°C), fourth column = low temperature (°C); fifth column = segment code.

Segment codes determine how the time-temperature path is generated between constraints. When defining inverse models interactively using the graphical interface, they are displayed in ovals along lines connecting the constraints (this is a good way to get a feel for what they look like). The format of the codes is:
<*Num times to halve*><*randomizer style*>[</*Max heating or cooling rate*>]
where:
Num times to halve is an integer from 0 to 5.
Randomizer style is E (Episodic), I (Intermediate) or G (Gradual).
Max rate is optional, is preceded by a slash (/), and is in units of °C/My.
Examples:

2I	Halve subsegments twice, use Intermediate randomizer.
3E/10	Halve subsegments 3 times, use Episodic randomizer, but ensure maximum heating or cooling rate of 10°C/My.

The final time-temperature constraint needs no segment code, and the beginning and ending times should be zero.

An example batch file follows in which two inverse models are run using a single HFT file and creating two new HFT files:

```
BatchType:  2
c:/testdata.hft
c:/test1.hft
Morrison on NW La Sal flank; 10000 tries
2     72    58
0     0     10000
4
95    70    200   200   1I
72    58    20    20    2G/5
```

```
60     25     170    70     3E/10
0      0      20     20
c:/testdata.hft
c:/test2.hft
Morrison on NW La Sal flank; 100 good
2      72     58
0      1      100
4
95     70     200    200    1I
72     58     20     20     2G/5
60     25     170    70     3E/10
0      0      20     20
```

Appendix D: Supplementary Information

D.1. Introduction

This Appendix contains miscellaneous information on details of certain calculations in HeFTy that are not detailed elsewhere in the manual, and are not described sufficiently in the literature to be easily reproducible.

D.2. Apatite Fission-Track Phi Method Calculations

What is called the "Phi Method" for apatite fission-track age calculations in HeFTy is described in detail by Jonckheere (2003). A simplified version of the age equation is:

$$t = \lambda_F^{-1}\zeta\left(\rho_s/\rho_i\right)I\phi\sigma\,,$$

where t is the age, λ_F is the fission half-life of ^{238}U, ζ is a zeta value quantifying mostly geometrical factors (see Jonckheere 2003 and references therein for information on how to calibrate this value), ρ_s/ρ_i is the ratio of spontaneous and induced fission-track densities, I is the isotopic ratio of ^{235}U to ^{238}U, ϕ is the corrected thermal neutron fluence for the reactor, and σ is the effective thermal neutron cross section of ^{235}U for fission.

The user enters the values necessary for ζ, ϕ, ρ_s/ρ_i and their uncertainties. The values for I and σ are hard-coded into HeFTy. The most conservative current value for I is 0.00725 ± 0.0005 (2 sigma). For formula for the thermal neutron cross section is:

$$\sigma = g\left(T\right)\sigma_0\,,$$

where σ_0 is the ideal cross section (586×10^{-24} cm^2 (Holden and Holden 1989)) and g(T) is a temperature-dependent correction for non-ideal 1/ν dependence of the ^{235}U fission cross section. Most reactor channels used for fission-track irradiation are in the range 20-60°C. The g(T) value for 20°C is 0.9832; for 40°C it is 0.9792; and for 60°C it is 0.9755 (Holden, 1999). HeFTy assumes a value of 0.979 ± 0.004 (2 sigma). The uncertainties in I and σ are incorporated into the age uncertainties calculated by HeFTy.