QTQt v 5.8.5 User Guide

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Introduction

QTQt is a program to infer thermal histories from low temperature thermochronology data using multiple samples. The name comes from QT being Quantitative Thermochronology and Qt (pronounced as cute or cutie) being the software used to develop the user interface. QTQt is currently implemented for apatite and zircon fission track, apatite and zircon (U-Th)/He data and vitrinite reflectance, and $^{4}He/^{3}He$ and $^{40}Ar/^{39}Ar$ age spectra. You can also enter you own kinetics for any mineral/isotope system combination (e.g. to simulate zircon (U-Th)/He or mica argon data, subject to the requirement that the diffusion domain can be treated as a single sphere, whose size, or equivalent dimensions of a rectangular crystal need to be specified also). It is also possible to specify the diffusion domain as an infinite cylinder or an infinite slab. Also, the current version allows for multiple sample modelling only if the samples under consideration have the same form of thermal history, i.e. can be treated as a vertical profile (see Gallagher et al 2005). You can still model a single sample, but for generality we will still refer to a profile (even if there is just one sample). A future version will include the 3D partition model-vertical profile approach developed by Stephenson et al. (2006).

For fission track annealing, the program uses the multicompositional algorithms of Ketcham et al (1999, 2007) and the original Durango apatite-based algorithm of Laslett et al. (1987) for predicting fission track annealing in apatite, and those of Tagami et al (1998) and Yamada (2007) for zircon. Currently, a given sample can be modelled with a constant composition (if appropriate). The composition could be taken as the average of measured single grain compositions or alternatively a single real sample could be divided up into multiple samples based on different compositions for example amd then treated as mutliple samples for modelling purposes. Similarly a sample with both apatite and zircon data should be treated as 2 samples, choosing the appropriate annealing model for each.

For predicting He diffusion, standard diffusion equations are used (typically a spherical grain with the same surface area to volume ratio as the dimensions specified for a real grain). You can input kinetic parameters to simulate He diffusion in any mineral (zircon for example). The He diffusion model also includes the recent developments on radiation damage trapping (Flowers et al. 2009, Gautheron et al. 2009, Willett et al. 2017, Recanati et al; 2017 for apatite and Guenthner et al. 2013 and Ginster et al. 2019 for zircon) using fission track annealing as a proxy to recalibrate the helium diffusion coefficient. It is possible also to include $^{4}He/^{3}He$ degassing spectrum as part of the He data modelling process.

A similar approach is used for $^{40}Ar/^{39}Ar$ spectra and the modelling routines incorporate the MDD method of Lovera et al. (1989, 1991). It is also possible to use the same routines for modelling diffusion in other systems, such as U-Pb in apatite and K-Ar (or Ar-Ar) in mica. This requires specifying the mineral and isotope systems either from a range of predefined values, or you can define a single parent-daughter pair by providing the appropriate decay constant, and diffusion parameters.

Vitrinite reflectance data can be incorporated, being used either as a direct constraint on the inferred thermal histories, or it is possible just to predict vitrinite reflectance and make a qualititative comparison to the observed values. The default algorithm is from Sweeney and Burnham (1990), equivalent to EasyRo, but the more recent IKU model of Ritter et al. (1996) and the basin%Ro model of Neilsen et al. (2015) is also available. Finally for $^{40}Ar/^{39}Ar$ age spectra, QTQT follows the MDD approach of Lovera et al. (1989, 1991).

The inversion scheme is Bayesian transdimensional Markov chain Monte Carlo (MCMC), in which the number of time temperature points (or the complexity of the thermal history solutions are inferred from the data rather than being specified in advance). The development of the method for

thermal history modelling is given in Gallagher (2012), and some other relevant publications are Gallagher et al. (2009), Charvin et al. (2009), Hopcroft et al. (2007) and Sambridge et al (2006). The approach as implemented in QTQt allows the user to specify one general time-temperature box, from which time-temperature points are sampled to construct a continuous thermal history by linear interpolation between the sampled points. It also allows for up to 5 additional time-temperature boxes to be specified to allow the user to add more specific constraints on the thermal history.

It is possible to select resampling schemes for the observed data, or the errors on the observations it it is considered they are not well known (or could be more noisy than the default values may suggest). This is sometimes referred to as Empirical or Hierarchical Bayes and examples of this are given in Gallagher et al. (2011).

When the program is actually running there is little to see (just a progress bar in the top level window). The results of the run are saved to a file (which is deleted when you quit the program, unless you choose to save it), and this summary file is used for generating a series of plots to examine the results once the run has finished.

QTQt was written in C and C++ by Kerry Gallagher (kerry.gallagher@univ-rennes1.fr), although some of the implementation of the fission track annealing algorithms is based substantially on subroutines provided by Richard Ketcham, and Rich's co-operation is gratefully acknowledged. The zircon radiation damage models are based on codes written by Willy Guenthner, and the Willett apatite radiation damage model is based on code written by Chelsea Willetts...thanks to them for providing their codes. Also, the main routine used for calculating $^{40}Ar/^{39}Ar$ spectra was adapted from code provided by Peter Zeitler (who adapted code originally written by Oscar Lovera), so they are thanked also.
We also acknowledge Qt (http://qt-project.org/) for providing such a professional programming environment for free. This software would not exist without them.

QTQt v5.8.5 has been built with Qt 5.12.3 and Qwt 6.1.2. It was complied with Clang x86 64bit on a Macintosh using OS X 10.14 (Mojave). The current version is 64 bit only and will run on machines with OS X 10.9 (Mavericks) or higher.

The current PC version was compiled with MinGW on Windows 10 and is also 64bit only (although it may be possible to produce a 32bit version if required). It has been tested on various operating systems (Windows 7, XP, Vista), but not extensively.

If you have problems with any version (i.e. it crashes), or suggestions for modifications then feel free to contact Kerry Gallagher. For a crash, try to give as much detail as you can concerning what you did and how it crashed. Also, send the data files you were using as that seems to be the most common fault. Some platform specific issues are highlighted in this documentation as ***PC USERS..*** or ***MAC USERS…***

However, read this documentation closely before trying to run the software on your own data – if it is not clear, please contact Kerry Gallagher, who is happy to change things to make them clearer.

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INSTALLING QTQT

If you are reading this you have probably already installed QTQt.

MAC USERS..

On a Macintosh the application QTQt is self contained.

PC USERS..

On a PC I have set up QTQt such that all the required libraries need to be in the same directory as the application itself. The default installation directory is "Program Files".

Note : When running, QTQt creates several output files in the directory where it running. Some versions of Windows do not have automatic write permission for the directory "Program Files", even if you are the adminstrator. This seems to be the case for Windows 7 and later. You can find some solutions by seraching the internet, or you can just install the software to a directory such as "Documents" where you have write permission.

The figures in this documentation are all taken from a version of QTQt running on a Macintosh, so may differ visually on a PC.
Using the Edit menu keys such as control-c option for copying or control-v option for pasting may not work on all versions of Windows. If not, you can use the copy or paste option directly from the edit menu.

DATA INPUT FORMAT

A typical input format required for QTQt is summarised in appendix 1 and a series of example data files are provided with the download. QTQt allows the user to input the data via the screen and this is the recommended method as there will be no problems with the format of the data files saved from the program, which may not be the case if you create the files using just a text editor (you do use a text editor, a word of caution – it is better if values entered on the same line are separated by a single space or tab only).

MAC USERS.. On a Macintosh, there have been problems with the default "end of line" character (which is invisible). Qt (the environment used to develop the user interface) apparently does not yet recognise the Macintosh end of line. This can be a problem with Excel and TextEdit for example. I have tried to pick this problem up when reading input files. However, if the program crashes when you open a file created with a text editor on a Macintosh, this is a likely explanation. You can use TextWrangler (the old BBEdit) and use save as with Unix "end of line "characters.
The example files included are

(i) QTQtexample.txt – this has AFT data and 3 AHe ages from a single sample with a simple reheating-cooling history
(ii) A series of 8 samples in a vertical profile - SynA1750HR.txt….to SynA0HR.txt with AFT data and 1 AHe age for each sample.

In appendix 2, there are examples of input and output for these 2 sets of data, so you can test these out quickly.

RUNNING QTQT

Having launched QTQt, you will see a menu bar over a main window as shown below :

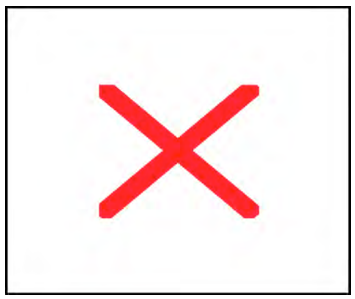
Required parameters are missing or incorrect.

Currently, the number of samples in a vertical profile is limited to 50.
You will also see your home directory listed and a series of run and plot options, that are stored in a file in you home directory. The first time you start QTQt, this file will not exist, but will be created.

The various menus are described as they appear on the menu bar. Note that some menu options are disabled until certain parameters have been set. If you try to run a different profile having already run another one, then many menu options enabled for the previous run will be disabled for the current one, until you set the appropriate parameters for the current run.

Since QTQt 5.4.2, there is selection in the Plotting menu that allows you to set some default parameters for running QTQt and these can be changed at any time. The latest choices will be loaded each time you launch QTQt and written to the main QTQt window.

This menu option (**QTQt run and plot options**) and the dialog window that will appear are shown below.



The options currently available are

(i) Select between pdf and SVG format for graphical output. Both are scalable vector formats, and can be edited with Adobe Illustrator for example. However, the pdf format that is selected by Qt produces files in which the text objects are treated as vectors (rather than editable text), whereas the older SVG format contains editable text. This pdf problem seems particularly the case for Macintosh. A second however, Adobe recently announced they will no longer support SVG.

(ii) Select between text and binary formats for some output files. The binary option leads to smaller files, and faster I/O, but will not be readable as text. However, the plots that will be written in binary are used just for plotting. The main QTQt output file will always be a text file.

(iii) Select the temperature axis to either increase upwards (as often preferred in Physics) or increase downwards (as often preferred in Earth Sciences).

(iv) Select the time axis to either increase to the right (as often preferred in Physics) or increase to the left (as often preferred in Earth Sciences). Time = 0 is the present day.

(v) Use temperature gradient for profiles...this lets you specify the temperature gradient (in °C/km) as a parameter for profile modelling. The default is to use the temperature offset. The two are related as temperature gradient = temperature offset/elevation range.

(vi) Select to base the axes on graphics on all data or only the data that is used for modelling (this is mainly for $^{40}Ar/^{39}Ar$ or $^{4}He/^{3}He$ spectra when some steps are flagged to not be used during modelling).

(vii) Select the default font style for annotating graphics.

(viii) Keep all graphics windows open...this will let you keep up to 20 graphics windows open at the same time to allow you to compare different aspects of the output more easily.

(ix) Allow plotting of all thermal histories. This allows you to plot a selection of 1000 hermal histories from the (post-burn-in) thermal histories accepted during the MCMC sampling ranked in terms of the likelihood or posterior probability. This appears as an option button on the toolbar when you plot selected thermal histories.

(x) Adaptive time step for AFT (apatite fission track). By default the time step used for AFT modelling is 1 m.y. (unless the time step between two input time-temperature points is less than 1 m.y.). For AFT modelling with the Ketcham et al. (1999, 2007) models, the adaptive time step option tries to speed up the calculation and calculates the equivalent time step to have a temperature step of

10°C for temperatures < 60°C
5°C for temperatures between 60°C
2°C for temperatures > 90°C

Irrespective of the default or calculated time step, there will always be a minimum of 10 calculation steps between two input time-temperature points.

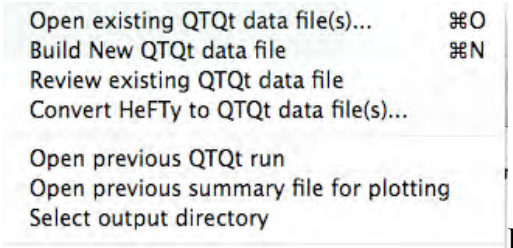
(xi) Default temperature steps for diffusion/radiation damage modelling. In trying to accelerate the calculation for diffusion (and radiation where appropriate), it is possible to define a default temperature step (and we then calculate the equivalent time step between 2 input time-temperature points). The diffusivity is taken as constant across that temperature step. This can particularly help speed up the calculations for long duration (deep time) thermal histories, in which there may be long periods at near constant temperature. As in (x), irrespective of the default or calculated time step, there will always be a minimum of 10 calculation steps between two input time-temperature points.

(xii) Plot axes defaults when generating all plots. This lets you specify a default range for the time and temperature axes when plotting all output (with the ***generate all plots*** option) so all thermal history plots will have the same axes. This is not applied when you produce plots manually by selecting specific options from the plot menu.

(xiii) Error rescaling factor range for He age and VR. Here you can select the range in scaling factor for the input errors if you have built (or modified) the data files to allow resampling of the input error. The maximum value is 1000 and the minimum is 0.001.

The options are saved to a file called .QTQToptions.txt, which is stored in your home directory. The file is hidden on a Macintosh.

FILE MENU



Required parameters are missing or incorrect.

Open Existing QTQt files(s)

This will produce a dialog window as below

Required parameters are missing or incorrect.

Clicking on **Open file** will produce a general open file dialog with a list of files in the current directory. The usual options will apply to selecting multiple files at once (e.g. on a Macintosh, using shift will allow you to select consecutive files in the file list, while shift-command lets you select mutliple files that are not consecutive in the the file list. Once you have selected one or more files from the first file list, another dialog box will appear allowing you to select another file using **Open another file**. You can keep doing this, and when you have selected all files for a particular run, you can select **Finish**.

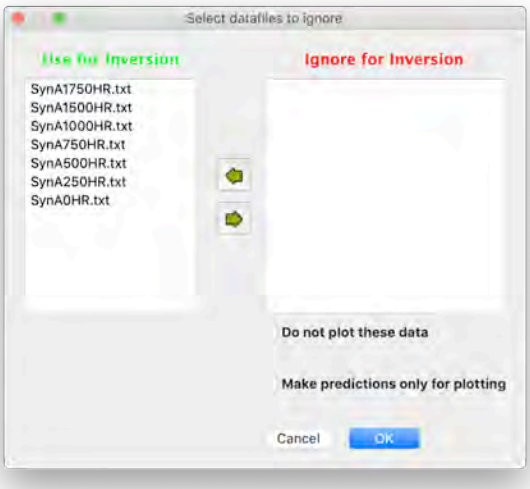
Required parameters are missing or incorrect.

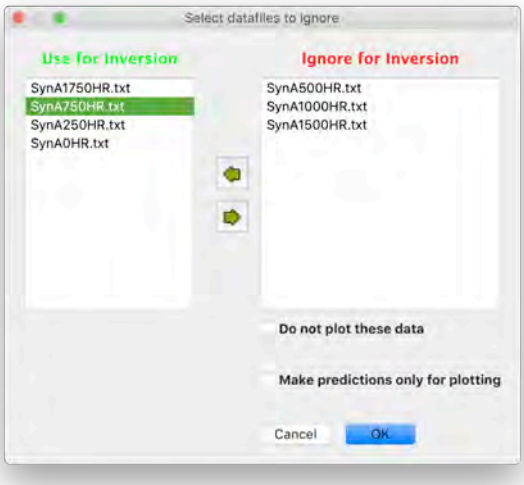
When you click on the finish button having opened just one file, or if you have loaded just one file from the previously opened file list at the bottom of this menu, the run title window will appear

Required parameters are missing or incorrect.

This lets you give a name or identifier to the current modelling run. This name is used for all output files and will appear on all of the plots subsequently.

If you have opened more than one file, as a vertical profile, the window on the left below will appear before the run title window.





You can selected files to ignore during inverse modelling, but you can still look at the predicted values for those data files. The data in the ignored files are not use to calculate the likelihood and so are not used in determining the thermal history models.

You can select each file and use to arrows to move from the left to right, or back, or just drag and drop the files you want to move. The window on the right above shows three data files selected to be ignored. You can select to make predictions just for individual thermal history model that can be plotted (max. likelihood, max, posterior or expected models). In this case, however, you can not look at the range of predicted values for the ignored data from all thermal history models, but the inversion will run faster as we will not be making predictions for the ignored data during the inversion run. Finally, there is also an option to not plot the data from the files selected (to be ignored). This lets you plot just the predicted values for those samples.

When looking at the thermal history results, those for the ignored files will be plotted in yellow.

If you add the word 'dummy' to a file name, that file will be automatically added to the ignore for inversion column. The word 'dummy' can be lowercase or uppercase, or a mixture of case. Dummy files are used when modelling detrital data as described later.

Once you click OK, the run name window will appear as described earlier. When multiple samples are used in a profile, sample specific data file will also have the sample's file name. This name is also used for a file with the appendix ".run" which will contain the filenames and thermal history modelling parameters, the last model sampled and the best model found during the current run. This can be reloaded as described below (so you do not have to enter all the parameters again).

Build QTQt data file

This menu option is discussed in detail later in the documentation.

Review existing QTQt data file

This allows you to load an existing QTQt datafile and edit it, using the same dialogs/windows as the build QTQt data file option.

Convert HeFTy to QTQt data file(s)

This converts some simple HeFTy text files to QTQt format. It will not work with binary files. At the time of writing, this has only been tested on fission track data (both EDM and LA-ICPMS formats). HeFTy age and length data files can also be converted when created a new QTQt data file when entering count and length data.

Open Previous QTQt Run

This allows you to open a file containing the filenames and thermal history modelling parameters, the last model sampled and the best model found during a previous run. This file will have the name of the modelling run (see Run Title above) and the suffix ".run". It is saved into either the directory where the QTQt application is located, or a user-specified output directory (see Select Output Directory below). If no name is enter, then the default is to save the information for the current run to a file called QTQt.run, in the current directory. Only files with the suffix run will be available to open. When you have selected to open a previous run file, you will see the following dialog window. This allows you to start the model run from the last model or best data fitting (maximum likelihood) model of the previous run, or start from a completely random thermal history model (but using the input parameters from the previous run). All parameters used in a previous run will be reused by

default in any subsequent run (including the values for time/temperature steps which can be set in the QTQt options)

Required parameters are missing or incorrect.
The run title window (described above) will appear after this window disappears. The window allowing you to select files to ignore will not appear when using the previous run option, as QTQt will already know which files to ignore.

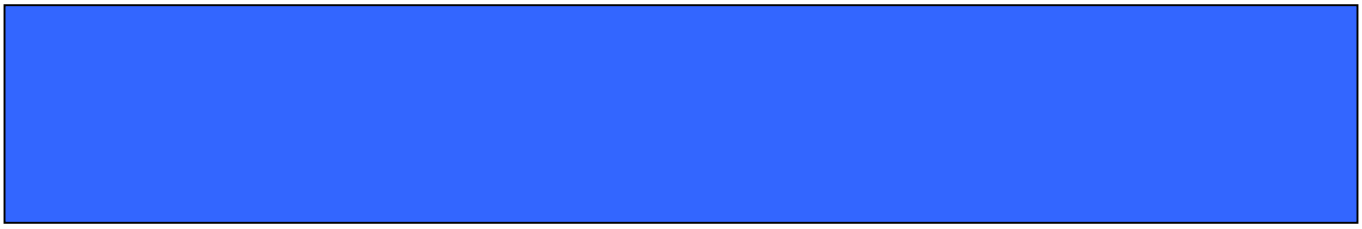
Open Previous Summary File for plotting
This lets you open a Run Summary file (as described above) to generate plots, if you decide you did not save ones you wanted previously.

If you have opened files previously with QTQt, you will have a list of previously opened files. This provides a short cut to open a single file. You can not open multiple files using this option.

Select output directory
This lets you select a directory where all output will be saved. The default is the directory of the last data file opened.

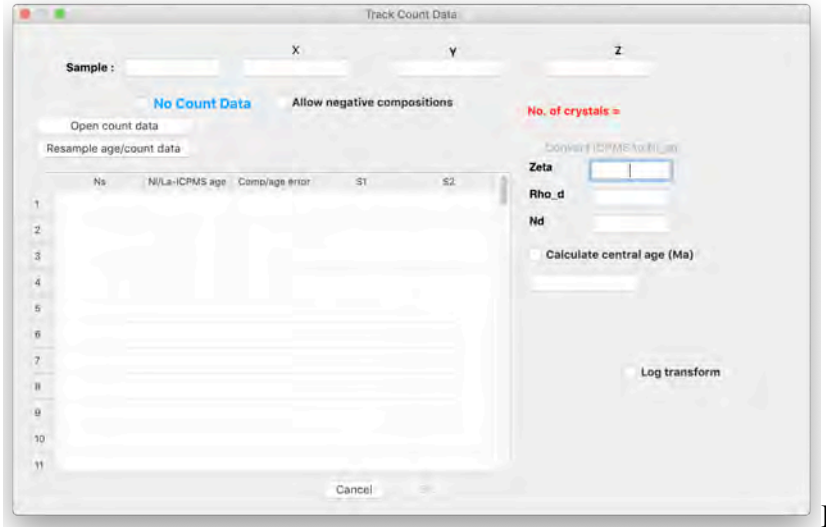
Build QTQt data file

This allows you to input FT single grain age counts, length data, (U-Th)/He age and vitrinite reflectance data for a given sample. You can optionally input track count and track length data, as well as some other specific information concerning a given sample and U-Th/He and vitrinite reflectance data, before being able to save the data to a file. Data files for $^{40}Ar/^{39}Ar$ and $^{4}He/^{3}He$ need to be created outside QTQt, and these are described later.



Fission track count data

The window below appears first.



Required parameters are missing or incorrect.

If you have no count data, then click on the **No Count Data** button. Otherwise, you need to enter a sample identifier (name), and the location information. The X and Y coordinates represent grid locations or longitude-latitude, but are not actually used in the current version. Z is the elevation in metres (enter negative Z for depth).

The check box **Allow negative compositions** can be checked to allow for compositional (or proxy) values to be negative. This can be the case when using calculated equivalent compositional values from rmro values for example. Contact Dale Issler at the Canadian Geological Survey in Calgary for more information.

You can use the **Open HeFTy count data** button, to select a HeFTy count data file, provided it is in the format defined as Age File, Traditional Zeta (see "HeFTy Import templates.xls" by Richard Ketcham). An example is below. The first line will be used as the default file name for QTQt, and when reading the file, QTQt looks for a line starting with "zeta" and another with "Ns Ni Dpar". At the moment, QTQt does not allow the HeFTy LA-ICP-MS fission track age data format.

Example of allowable HeFTy input count file format

QTQtTest
more info
whatever, up to 20 lines
Codes for kinetic parameters are: Dpar, Cl(wt%), Cl(apfu), OH(apfu), and rmr0
For ZFT, remove kinetic parameter column (Dpar in this example)
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

It is common to want to use old data from published papers, for which the full data set is not available. You can use the **Resample age/count data** button to produce a set of spontaneous and induced track count pairs ($\mathbf{N_s}$, $\mathbf{N_i}$) based on resampling from a given total sample (mean) age and error, and the total number of induced and spontaneous track counts and/or the total spontaneous/ induced track density ratio. Clicking on this button will produce the window shown below

You need to enter the sample age and error, and at least either the total number of spontaneous and induced tracks (**Sum(Ns)** and **Sum(Ni)**), or the total spontaneous/ induced track density ratio (**rhos/rhoi**). You can leave the other fields blank if you do not know the appropriate values and QTQt will use default values or estimate values based on the other input data. In this case, the resampling defaults are **# crystals** = 20 crystals, **zeta** = 340, **∂zeta** = 5, and appropriate values for **rhod**, and **Nd** are then calculated from the input age and error values. If you do not input **Sum(Ns)** and **Sum(Ni)**, these will be calculated using the input value of **rhos/rhoi** and assuming the total

number of spontaneous and induced tracks = 1000. If the ratio of **t**he input values, **Sum(Ns)/ Sum(Ni)** is not consistent with the input value **rhos/rhoi** , then QTQt will use the **rhos/rhoi** value for **Sum(Ns)/ Sum(Ni)**, under the assumption that perhaps different areas were used for the counting.

The parameter **resampling Ns+Ni** is to allow for some more realistic variation in the resampled data. If we use the same (average) Ns+Ni value for each crystal, then the resampling will tend to produce relatively less dispersed count data than real data (you can test this yourself by comparing the resampled values using the age, error and total counts for real count data to the actual counts and single grain ages). This is because we are effectively assuming all crystals have pretty much the same uranium content. By setting the resampling parameter to a value > 0, we can introduce more variation. The default value for this parameter is ±0.5 (of the mean Ns+Ni value), and the minimum is 0, and the maximum is ±0.95. If you know the $\mathbf{p}(\chi^2)$ value for the real data, you could adjust this parameter to obtain a similar value (the $\mathbf{p}(\chi^2)$ is shown just below the calculated central age). A higher value for the sampling range will tend to lead to more dispersed age data, but it will be generally be difficult to produce a set of count data with a very low $\mathbf{p}(\chi^2)$ value, as this implies the counts were not statistically consistent with a single population.

The resampling is done as follows : for a given crystal, we can choose value of Ns+Ni (selected randomly from a specified range, the default being 0.5 to 1.5 times the average Ns+Ni value (=(**Sum(Ns)** + **Sum(Ni))/ # crystals**). Ns is then obtained by sampling (given the value of Ns+Ni) from a binomial distribution, and then Ni can be calculated. This resampling for the specified number of crystals is repeated up to 100 times (or until the predicted age and error are within 1% and 5% of the input values). The resampled data that agree best with the input age and error will then be inserted into the input table.

You can manually enter the spontaneous and induced track count pairs ($\mathbf{N_s}$, $\mathbf{N_i}$) and compositional parameter for a given sample, or these can be cut from an standard application such as Excel by placing the cursor in the first row of Ns and pasting them into the table. The copy-paste option is the easiest.
If you find that the values do not line up in two columns, then it is because the character(s) between the Ns and Ni values in the original file are not a single space or a tab. The simple solution to this is to replace what ever that character is with a single space.
You can enter columns individually or all together.

PC USERS… using the control-v option may not work for pasting, but you can use the paste option int the edit menu to do this.

The title of the second column is **Ni/LA-ICPMS age**. This allows you to input either the number of induced counts (Ni)/ or LA-ICPMS ages, rather than Ni. In the first case (with counts for Ni), you can add a compositional measure for each pair of counts in the 3rd column. If you input LA-ICPMS ages, then the third column must be the error (1σ) on the LA-ICPMS age, and you ***must*** have compositional data which goes in the 4th column. (QTQt distinguishes the 2 types of input based on having either 3 or 4 columns of input). When inputting LA-ICPMS ages you can input all or some of the other parameters such as **Zeta**, **Rho_d** and **Nd**; Once you click on the **Convert ICMPS to Ni_eq** checkbox, QTQt will estimate the equivalent Ni (which may not be an integer value) based on the input values for **Zeta**, **Rho_d** and **Nd**. Alternatively it will either choose or estimate values for any parameters not entered, by trying to replicate the input errors as closely as possible. You will see that

the title of the 2nd column will change once the equivalent Ni values are calculated. The calculated single grain ages and appropriate 1 sigma error will be written to the 4th and 5th columns.`

As from version 5.4.5, QTQt can deal with 0 counts for Ns (which lead to a zero age) when using ICP-MS age and error data. QTQt will assume the age error is equivalent to the upper 95% confidence limit (and the lower confidence limit is the zero age), given by equation 3.22 in Galbraith (2005). Knowing this value allows us to estimate Ni for a grain with Ns = 0.

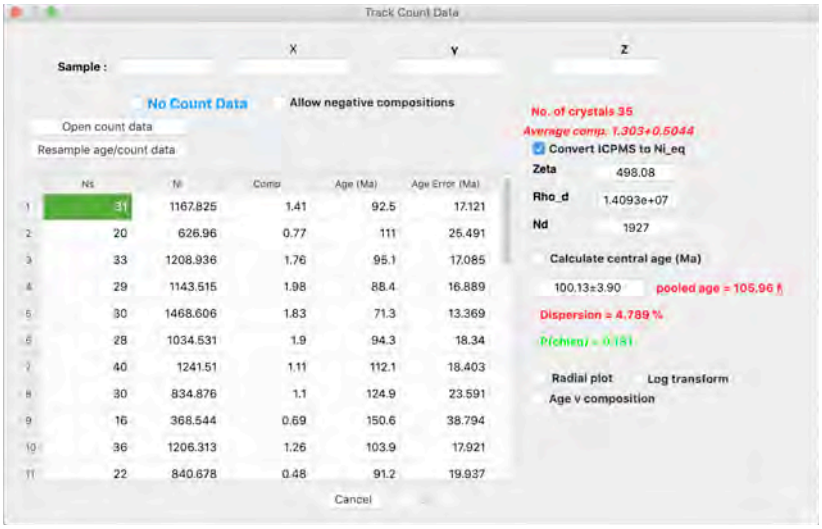
An example of input for LA-ICPMS ages is given below (you do not put in the column headings though)

Ns	ICPMS age	1σ	ClWt%
4	33.0	16.64	0.07
10	44.6	14.39	0.02
24	53.2	11.37	0.29
8	44.1	15.88	0.24
6	74.1	30.69	0.11
24	39.0	8.35	0.09
18	31.1	7.61	0.06
7	38.2	14.67	0.18
6	32.5	13.48	0.17
17	26.6	6.68	0.00
10	76.4	24.70	0.45
12	59.8	17.73	0.37

The 3rd/4th column (labelled **Comp)** allows you to input compositional data for individual grains in the same data file and this can be actual compositional data (e.g. Cl Wt %) or proxy data such as Dpar. In practice the average compositional value, taken as the mean of all input values (for both age grains and track length measurements) will be used for all calculations for a given data file, and this will be written on the Counts dialog window. If you enter some counts with no compositional value, then QTQt will assign the average compositional value to those data.

Finally, you can input **Zeta** (the analyst specific calibration factor used in the External Detector Method), **Rho_d** (the dosimeter track density) and **Nd** (number of tracks counted in the dosimeter).
If you do not have values for some or all of these parameters, you can leave the boxes blank, and QTQt will try to estimate reasonable values.

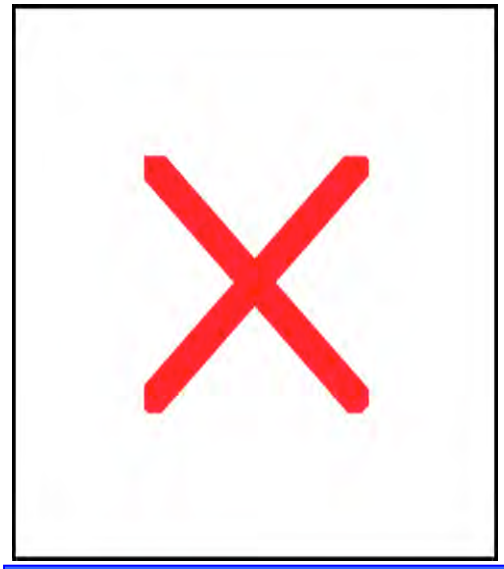
Once you have enter zeta, Rho-d and Nd, the central age will be calculated, with the χ^2 probability for the population. The 4th and 5th columns will have the single grain age and single grain age error for each grain, as below.



Having input the count (or equivalent) data and calculated the central age, you will also have the possibility to look at single grain age v composition, or age v age. This allows you to group the single grain age data in terms of composition or age ranges. If we select **Age v composition**, then you will have a graph (on the left in the image below). You can then use the mouse to group the single grain ages in terms of compositional ranges. You just need to hold down and drag the mouse over the compositional ranges you want. The groups will be colour coded both in the graphic (on the right in the image below) and in the count data table. The central age and χ^2 probability will be written next to the symbol for each group.

You can use the button Plot Age v Age to toggle between the age v composition and age v age plots. Again you can use the mouse to select the age ranges you want.

You can use the **Radial plot** check box to look at the radial plot which will also be coloured coded according to the groups selected. Once selected, the radial plot will automatically be updated if you modify the groupings and click anywhere on the input counts window.



Note : You can only group the ages on either composition or age, but not both.
Compositional groups :
The main reason for grouping on composition is that we can then use the appropriate compositional parameter in the fission track annealing model for each group. In this case, the compositional groups will be saved to the single data file you create.
Age groups :
The main reason for grouping on ages is that we can allow different thermal histories (particularly for provenance related thermal histories in sediments). If you group on age ranges, then QTQt will create separate data files for each age group using the same basic name, and adding the numbers 1, 2, 3, etc..according to the number of groups.

Fission track length data
The next window allows you to input track lengths, and other length relevant data for a given sample. The window below appears.
Required parameters are missing or incorrect.

If you have no length data, click on the **No Length Data** button. Otherwise, if you have already input information concerning the sample identifier and location, this will appear automatically. As with age data, you can cut and paste values for the length and angle (and the same caveat applies about generally having a single space between each value). You can input just length measurements or lengths and angle to c-axis data (and in this case you can choose to use a project track length annealing model or not – see Ketcham et al. 1999, 2007). As with the age data, the **Comp** field allows for individual compositional data for each track length measurement and the mean value will be calculated (and output to the final data file). If you enter some lengths with no compositional value, then QTQt will assign the average compositional value to those data.

Selecting the check box **Verify compositional bins** will check that the compositional data for track lengths falls into the same ranges as defined for the count data. If there are length compositional data outside the count compositional data range, then QTQt will add 1 or 2 extra compositional groups (either at the lower or upper end of the count compositional range, or both).

You can use the **Open HeFTy length data** button, to select a HeFTy length data file, provided it is in the format defined as Length File, without Lo (see "HeFTy Import templates.xls" by Richard Ketcham). An example is below. The first line will be used as the defaul file name for QTQt, and when reading the file, QTQt looks for a line with "length angle Dpar"

Example of allowable HeFTy input length file format

QTQtTest
more info
blah
blah

length	angle	Dpar
7.2	34	2.31
11.2200003	14.23	2.22
13.319	68.2	1.87

Select **Use projected tracks** to use a projected track length model, obviously this makes sense only if you have put in angle information, or you have previously transformed length data into c-axis equivalent lengths (not using projected tracks is the default). If you check this box, then you will see the mean track length for both projected and unprojected tracks.

Select the appropriate **Etchant** (5 M is the default).

Select **Cf tracks** if your sample used Cf irradiation to increase confined track revelation (the default is no Cf tracks).

If you want to return to the Counts data window, click on that button.

Binned track length data

Binned length data can be input (along with compositional information), ideally when you have the mean track length (MTL) and standard deviation (SD) of the binned distribution. QTQt will then generate a set of individual tracks lengths with the same statistics (histogram bin values, MTL and SD) as the inout values.

There are two way to enter binned length data, manually or from a file.

(i) Manual

You need to first enter the MTL and SD values in the appropriate boxes. You can continue without these values, but you will see a warning dialog, stating that QTQt will estimate the MTL and SD, but it is better to put them in.

Then you can enter (or paste) the binned length distribution data into the table. You can paste 2 or more columns into the table : the first column is the value of the length for each bin, and this must have 20 values from 1 to 20 microns. The second column in the number of tracks in each bin (use 0 if there are no tracks in a given bin). The third column can be used to input the composition or compositional proxy (this should be the same in each bin).

If you have just the bin counts (i.e. no compositional data), then you can just paste the 20 bin counts into the first column (provided you have already entered the MTL and SD values) and no need to use the bin vaues (from 1-20)/

(ii) From a file

This option is aimed at data in the format typically reported by Geotrack, where the data are often sub-divided into compositional groups of 0.1 Wt% Cl. You need to create a text file, with values separated by a tab or space(s). An example of the structure of this file is given below :

```
0.0 0.1 9.8 3.1 0 1 7 3 3 3 2 5 11 19 27 23 10 6 3 3 0 0 0 0
0.1 0.2 9.0 3.4 0 1 2 3 1 0 1 1 4 4 8 7 1 2 1 0 0 0 0 0
0.2 0.3 10.0 1.8 0 0 0 0 0 0 0 2 3 4 1 1 3 0 0 0 0 0 0 0
0.4 0.5 11.0 0.7 0 0 0 0 0 0 0 0 0 0 0 2 2 0 0 0 0 0 0 0
0.7 0.8 12.1 1.5 0 0 0 0 0 0 0 0 0 0 1 5 6 3 3 3 1 0 0 0
1.3 1.4 12.6 0.9 0 0 0 0 0 0 0 0 0 0 0 1 2 1 0 0 0 0 0 0
```

The first 2 terms are the compositional range for the length data to follow. This needs to be Cl content in Wt% and these need to be in 0.1 Wt % intervals (but not necessarily continuous, as shown above with the jump from 0.7-0.8 to 1.3-1.4).

The next 2 terms are the mean track length and the standard deviation of the length data for this compositional range.

The next 20 values are the number of track lengths in each bin (at 1 micron intervals) from 0.0-1.0 to 19.0-20.0 microns.

As implied from the example, you can enter multiple compositional bins in this way, using just one file.

Having enter binned data, you will see then that QTQt produces a set of individual length values (with a C-axis angle left blank). This is generated by sampling the binned distribution to give set of

lengths will have the same binned distribution and (more or less) the same mean and standard deviation as the input values.

If you have input compositional (or proxy for composition) data for the counts and/or lengths, then the average composition will be calculated using all the input values (that is, the reported average will be the weighted mean).

Note : The fission track annealing models for apatite generally require some compositional parameter to be specified. If you do not enter any compositional information for the fission track data at this stage, then you need to do this later when you come to save the file.

Compositionally binned count and length data

Sometimes, apatite fission track data for a given sample are presented divided into several compositional bins for both lengths and counts (or ages). QTQt can be used to model each compositional bin with the same thermal history. As described above, you can input length data from different compositional bins directly from a file you need to create (see above - ***From a file*** – for the format required) and if you have input all the count data using different compositional values, then you can just save the file (as described later).

Note : In general, QTQt will allow you to check that all the count and length data have been assigned to compositional groups. If the groups defined on count data do not include compositional values contained in the length data, QTQt will adjsut the groupings so that they do. This may involve QTQt adding one or two new groups, or just changing the ranges.

However, if you have already grouped age data according to composition, QTQt will assume you will not want to group the length data by opening a file containing binned compositional data as described above and (this option will not be available in the length data dialog).

Otherwise, you can do this manually. You need to do some manual text editing and there are 5 steps.

(i) Create a series of individual data files inputting the counts and lengths for each compositional bin (see above – ***Manual*** - for binned length data on how to create a set on individual length values from the binned values)

(ii) If you have created separate files, then you need to use a text editor to create one large file with all the data for that sample by pasting in the counts and lengths from each individual file.

(iii) Change the number of lengths and counts in this data file to make sure the values are equal to the input values. These are the 2nd and 3rd values on the 3rd line of the data file (see appendix 1 for a description of the typical data file).

(iv) **Insert a minus sign in front of the composition code parameter** (1st value on line 5 of the data file).

(v) After line 5 you need to insert the following information :
(a) The number of composition bins

(b) In order of increasing bin value, the lower and upper values defining the compositional bin (the modelling will use the average value of these two values).
For example, with 3 bins for Wt% Cl with values of 0.0-0.1, 0.1-0.2, 0.4-0.5, we would add

3
0.0 0.1
0.1 0.2
0.4 0.5

Then save the file. This can be opened as any QTQt data file for running, but note it will take longer than using a single composition sample to run the inversion as QTQt runs a forward model for each compositional bin, using the average of the upper and lower values for each bin as the compositional parameter. The data fit (likelihood) is calculated for each compositional bin data set, and these are summed to give the likelihood for the sample as a whole.

An example file is given below with the major differences to a standard data file shown in red and explained in the right hand column. See also appendix 1 for an explanation of the general data format.

CompBinsExample	
0 0 -2730.	
0 10 6 374.1 1.861e+06 43135	
105	
-3 0.05 0.0	The negative sign (-3) indicates we are using binned compositional data. The 3 indicates Cl Wt% as compositional parameter.
4	Number of bins
0.0 0.1	Lower limit, upper limit of bin 1
0.1 0.2	Lower limit, upper limit of bin 2
0.2 0.3	Lower limit, upper limit of bin 3
0.3 0.4	Lower limit, upper limit of bin 3
1 16.3	
0	
0	
1	
34.3 2,7	
12.13 1.56	
1.34 0.134	
0 32 0.0000	Count data....Ns, Ni and composition of grain 1
2 136 0.0700	Count data....Ns, Ni and composition of grain 2
0 48 1.4000	.....etc
14 497 2.7000	
3 145 2.9000	
0 243 3.3000	
10.34 0.32	Length and composition of the host grain...
11.56 0.36	.....etc
10.51 0.22	
13.06 0.21	
9.72 0.17	

12.01 0.19	
12.13 0.03	
12.45 0.07	
13.61 0.02	
12.81 0.09	

Note when plotting FT ages and MTL for multicompositional samples against the predicted values, the default is to plot the appropriate values for each compositional bin for each sample. This can get a little cluttered, so there is also the option to plot the mean values for a given sample. In this case, the values plotted are the weighted means, weighted by the number of counts (or track lengths) in each compositional bin. For the FT age, this weighted mean age is generally not the same as the central age, calculated from from input Ns and Ni values. For the modelling, it is the Ns and Ni values that are used (in the likelihood calculation), while the weighted mean is just for graphical purposes/visual comparison.

Diffusion models

U-Th/He (and other diffusion systems) data, Broken crystals, U-Th zoning, $^{4}He/^{3}He$ data, $^{40}Ar/^{39}Ar$ data, and Single crystal age profile data.

To incorporate (U-Th)/He data (or any single domain diffusion type data), the window below will appear.

If you have no U-Th/He data, click on the **No He Data** button. Otherwise, you can enter just the observed age (**Uncorrected age**) and **Error**, or if you want to calculate the age you can enter the U, Th, Sm and He concentrations (in the units indicated on the window) and click the **Calculate Age** button. Note for helium ages, the input is the *uncorrected* (for alpha ejection, or Ft) age. The uncorrected He age will be compared to the input age. If these are not equal, and the He ejection distance is not zero, then by default, the input age is reset to the calculated age for consistency. If you calculate the He age, then the Ft-corrected age will be written in red to the right of the uncorrected age.

If you want to use Monte Carlo sampling of the observed He age (using a normal distribution, centred on the observed value, with a standard deviation equal to the input error), you can check the box **Resample He age with MCMC**. Instead of trying to fit just the single input age, this process samples the normal distribution, allowing for the uncertainty in the observation. In practice this can be thought of as a way of allowing for uncertainty in the predictive model (e.g. the kinetics), in that we do not try to fit the observed age exactly. This option is indicated in the data file by a minus sign in front of the input age.

Alternatively, you can select **Resample He Error with MCMC**. This option samples a scaling factor for the input error, which is used in the calculation of the data fit. The scaling factor is between 0.1 and 10 so the data can effectively be treated as being more precise (low scaling factor) or less precise (high scaling factor), relative to the input error value. This may be useful when you are not sure of

how good you error estimates are. When you set the MCMC parameters (described later) this is controlled by the **He Diffusion** proposal scale parameter. When you save the data file, you will notice that the either He age or the He age error will be a negative value – this indicates that you will use this sampling approach (varying either the age of the error as described above). This option is indicated in the data file by a minus sign in front of the input error.or

If you wish to ignore a particular age for inverse modelling, you can select **Ignore this age for Inversion**. In this case, the predictions will be made for this age, but not used in the likelihood calculation, so will not influence the sampling of thermal history models. This option is indicated in the data file by a minus sign in front of both the input age and the input error.

Note : You can not choose to vary both He age and He error for samples in the same run. If you have a mixture of these 2 possibilities in a data file (or even both for the same analysis), QTQt will default to sample only the He error for those ages that have just the sample He error option selected.

You can input values for **U**, **Th**, **Sm** (usually in ppm, but other choices are available) and **He** (usually in ncc/gm, but other choices are available) or you can leave these blank. If you input these values, then QTQt can calculate the age, but in general it is recommended to input the age calculated elsewhere.

Note QTQt will check the input values and if these are greater than 1000, it will assume these are concentrations in atoms and will calculate an equivalent ppm (or ncc/gm for He) using the total mass estimated from the input dimensions for the crystal (see below), using a density of 3200 kgm^{-3} for apatite or 4650 kgm^{-3} for zircon.

IN ALL CASES THE OUTPUT IN THE DATAFIULES WILL HAVE CONCENTRATIONS FOR U, TH AND SM IN PPM, AND NCC/GM FOR HE

In terms of the minimum information you need to input, this will be the observed age, its error and the grain size. Note the default mineral is apatite, and the default grain geometry (for the model calculations) is spherical. If you want to use a radiation damage model, then you will also need to inout at least a value for U concentration (if value for Th is not input, QTQt will assume the input U value is the effective eU value).

You can select the mineral/isotope system type (apatite, zircon, K-Ar/Ar or other) and if using radiation damage models for apatite and zircon, the default diffusion parameters will be inserted into the appropriate fields. For K-Ar/Ar the default mineral is mica, but you can override the default diffusion parameters is you need to. If you want to simulate U-Pb ages in apatite for example, you just need to input the appropriate diffusion parameters (Do and E) and make sure the alpha ejection distance is set to zero. You may also want to select a different mineral geometry to the spherical default (described below).
If you want to simulate the age for another decay system, you can select other. You input the decay constant (in inverse seconds) in the field for alpha ejection distance, and QTQt will use that value for the difussion-production calculation (and of course the actual alpha ejection value will be zero for those calculations).

Also you an select the crystal geometry for the diffusion calculation, choosing through the **Geometry** dropdown menu, from **sphere**, **infinite cylinder**, **infinite slab** or **fragment** (see below for fragment/broken crystals). Some choices will lead to a default selection for the geometry (e.g. He in apatite and zircon will always be a sphere) . Also, selection of specific geometries will change the headings in the dimensions parameters (described below). For the cylinder and slab, we require just one parameter for the dimension (either radius or thickness).

For the diffusion calculation, you need to enter the dimensions of the grain. In QTQt we use the long axis (**length**), and the other 2 axes (**width, thickness**). In terms of the calculation, a sphere is used by default, and its radius is calculated from the three input dimensions, under the assumption that the sphere has the same surface area to volume ratio as a rectangular grain. If you enter the **thickness** as zero, then it is assumed that the width and thickness are the same (and we use the width value for both). If you enter the **width** as zero, then it is assumed that the length is the radius of a spherical grain. As you enter the crystal dimension, you will see the equivalent radius of a spherical grain written to the right of the thickness box. As mentioned above, the choice of infinite cylinder will leave you with just the option to enter the **radius**, and the infinite slab, the **thickness**.

Resampling the equivalent spherical radius.
For the mineral selected as other (see below), it is possible to resample the equivalent spherical radius. This can be useful for minerals such as iron oxides that may have diffusion domains that are not the same as the grain size, but have not been estimated (as we can do with step heating experimenbts for example). This resampling requires you select an initial value and a range defined by minimum and maximum values. You enter these as the length, width and thickness parameters respectively. The sampling is done uniformly on a log10 scale, and you can choose to sample either randomly by drawing independent values from the specified range, or using conditional sampling such that the proposed new value is a perturbation of the current spherical radius value for a grain. You can choose between these two options by setting the value for **Resample eU** (see below) to either -1 (random uniform sampling) or -2 (conditional sampling). The accepted distributions of the sampling can be examined with the same plot as we would use to look at resampling the ages or errors. This resampling can not be done at the same time as resampling eU, the age or the error.

By selecting a shape under the **Geometry** dropdown menu you can override the default geometries.

Fragment/Broken crystals
Following the model proposed by Brown et al. (2013) and Beucher et al. (2013), it is possible to deal with broken crystals. This can be implemented for apatite with 1 termination or 0 terminations, the 1T and 0T crystals of Brown et al. 2013). This is done by selecting **1T fragment** or **0T fragment** or from the **Geometry** dropdown menu. The calculations are made by approximating the original crystal as a finite length cylinder with hemi-spherical terminations with the same radius as the cylindrical part of the crystal, as shown below.

The initial unknown length is L_0, the actual fragment length is L_f, the radius of the hemispherical terminations and cylindrical core is R, and the length of the cylindrical core is L_c. The ? indicates a missing part of the original crystal for 1T and 0T grains.

The minimum initial total length is defined by the length of the finite cylinder and 2x the radius. The actual total length is unknown, but it can be specified by the user (see notes below). However, its value is generally not too important provided it is large enough. For a given broken crystal segment, we need to enter the measured length of the broken crystal segment in the **length** field, and the thickness or diameter (2x the radius) of the cylindrical portion as the **width**. For a 1T grain, the width is written to the data file as a negative value and for a 0T grain, it is both the **length** and the **width** that written as negative values to the data file. The negative signs flag a broken cylinder (1T or 0T) for calculations. You can also enter a value for the **thickness** dimension and QTQt will then calculate an effective radius for the cylinder (by keeping the surface area to perimeter ratio for the cylindrical cross section the same the rectangular cross section).

When entering values for 1T and 0T grains, you may notice the heading **width** changes to **diameter**, and the **thickness** heading will disappear. This assumes that if there is no value enter for **thickness**, then the value given for width will be the diameter, as described above. However, if you enter a value for **thickness**, then headings will be reset to the original setting.
In the current version of QTQt, we deal with a 0T grains as for a 1T grain as above, but later you will need to explicitly edit the data file and insert a minus sign before the **length**. (see below)

The modelling with broken crystals or fragments tries to replicate the spread in single grain/fragment ages for a given sample, by predicting the range in ages from a whole (long) grain down to the shortest observed fragment size for a given thermal history.

Note : when you run models with 1T or 0T fragments, you will see a window asking you to choose either a fast method for modelling or a slower, more complete method, as below.

Both methods based on a finite difference scheme for diffusion in a cylinder. The fast method assumes diffusion at high temperature or high diffusivity will always completely degas a crystal. If this is not the case, then the final calculated age will be younger than that calculated with the more complete method. However, it is much faster than the complete solution. If you choose to use the faster methods it is recommended to check the final models (e.g. maximum likelihood model, expected model) with the complete solution, to assess whether this is a problem or not.

Below is an example of the input line for helium age data (see appendix for more detail) with notes regarding how to implement broken crystals/fragments.

11.35 32.61 106.51 0.0 51.4 3 **160 45 38**	The last 3 values in bold are the crystal dimensions of **length**, width and thickness. These dimensions are for a whole (**2T** crystal).
11.35 32.61 106.51 0.0 51.4 3 **160 -45.6 0** 11.35 32.61 106.51 0.0 51.4 3 **160 -45.6 38** 11.35 32.61 106.51 0.0 51.4 3 **160 -45.6 -300**	(i) The minus sign in front of the width indicates this is a **1T** fragment, and the length is the fragment length, the width is equivalent to either the width or the diameter (x2 radius) of a cylinder. (ii) If the, thickness is 0 then the 2nd dimension is treated as a diameter. (iii) If the thickness is > 0 then the grain has a rectangular cross section, and QTQt will calculate the equivalent radius of a cylinder with the same perimeter to area ratio as the rectangle. (iv) If the, thickness is < 0 then this dimension is treated as the initial length of the unbroken grain for modelling purposes. The 2nd dimension is then treated as a diameter.
11.35 32.61 106.51 0.0 51.4 3 **-160 -45 0** 11.35 32.61 106.51 0.0 51.4 3 **-160 -45 0** 11.35 32.61 106.51 0.0 51.4 3 **-160 -45 -300** 11.35 32.61 106.51 0.0 51.4 3 **-160.075 -45 -300**	(i) The minus sign in front of both the length and width indicates indicates this is a **0T** fragment, and the length is the fragment length, the width is equivalent to either the width or the diameter (x2 radius) of a cylinder. (ii) If the thickness is 0 then the 2nd dimension is treated as a diameter. (iii) If the thickness is > 0 then the grain has a rectangular cross section, and QTQt will calculate the equivalent radius of a cylinder with the same perimeter to area ratio as the rectangle.. (iv) If the, thickness is < 0 then this dimension is treated as the initial length of the unbroken grain for modelling purposes. The 2nd dimension is then treated as a diameter. (v) if there are numbers after the decimal point in the length, then these (x 1000) are used to indicate as the location of the 0T fragment relative to the left hand end of the original complete crystal, which is assumed to be given by 3 numbers, XXX, for a value between 000 and 999 microns) . In the example to the left, the length of a **0T** fragment is specified as **160.075**, but it has an actual length of **160** microns, and is assumed to have its left hand end located 75 microns (=0.**075** x 1000) from the left hand end of the original complete crystal.

Comment on 1T and 0T fragments

The current implementation for 0T grains uses the fact that although we have the fragment length, in general we do not know where in the original grain the fragment is from. This creates a problem for inverse modelling when trying to compare the observed fragment age to a predicted age - which predicted age do we use ? The range of possible ages for a fragment of a given length is predictable, as indicted in the figure below for different length 0T fragment taken from different parts of a crystal.

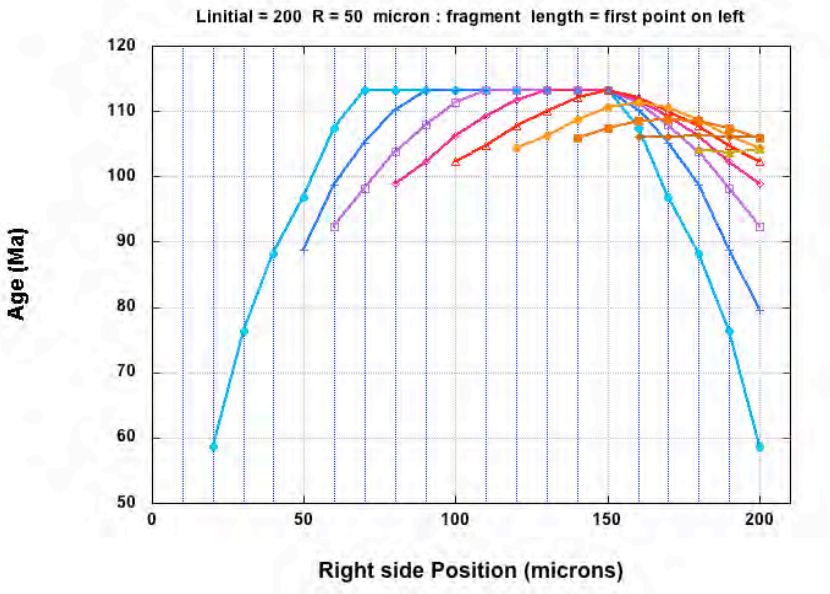


Figure showing the predicted age of a 0T fragment as a function of the fragment length and the original position of the fragment in a crystal of 200 microns length. Each curve is for a given length 0T fragment whose length is indicated by the first point on the left of the curve relative to the origin (and this first fragment is effectively a 1T fragment taken from the left hand side of the original crystal). Note how the range of possible ages reduces and tends to produce realtivly old value as the ratio of radius to fragment length reduces.

It is therefore straightforward to define a maximum and minimum age for a given 0T fragment with the youngest age being no younger than a 1T fragment of the same length, and the oldest age being from the centre of the original crystal, with no contribution from the terminations. When using 0T fragments in an inverse model, we set the predicted ages to the minimum or maximum possible value if the observed age is outside this range. If the observed age falls in the predicted range we could randomly select the predicted age from within this range to compare to the observed age. Alternatively, we could just set the predicted age to the observed or a value given by the observed age with some Gaussian noise added (based on the input error for the observed age, as the observed age can be considered a random realisation of the true age). Version 5.6.0 of QTQt has the last option implemented as it is the most optimistic approach for sampling a wider range of potential thermal histories. As we will generally not know from where in the original crystal the fragment is from, provided a 0T grain has an age that falls in the predicted range, the thermal history is consistent with the age of the 0T grain. All thermal histories that are consistent with the 0T grain should be treated (more or less) equally, and it would be up to information from other data to discriminate between them.

We adopt a similar approach for a 1T grain, in that we can define maximum and minimum ages. The maximum is the case when the 1T fragment length is considered to be the total crystal length minus

the length of a termination. The minimum length is that calculated for the 1T termination with a much longer initial length. The default for this initial length is x3 the fragment length.

When generating synthetic data or running a forward model in which we specify the initial length of the crystal and, for a 0T fragment, the position in the crystal the fragment is from, the age returned will be set to the actual predicted value for each fragment. That is, any input observed age will be ignored, and no noise will be added to the predicted value.

For the case of running a forward model in which we want to ignore any input age data, but have not specified where in the grain a 0T grain is from, the age returned is a value drawn at random from the range defined by the maximum and minimum values. We use a cumulative hazard type distribution, which will tend to bias the sampling towards older ages when the radius/fragment, R/L_f , is small, as we can anticipate the 0T fragment is more likely to come from the cylindrical part of the total grain and so have an older age. This approach is purely empirical but does broadly capture the behaviour seen earlier in the figure above. In practice we probably should consider the initial length of the grain, but as this is not known we do not deal with this parameter at present. We would expect the probability of sampling an older age (from the cylindrical part of the crystal) to increase as the initial length increases for a fixed radius.
We define

$$\alpha = 1 - \frac{R}{L_f};\ \beta = \frac{1}{1-\alpha};\ x = 1 - \beta^{-u}$$

Then with a uniform random number, *u*, we sample the predicted age as

$$age = age_{\min} + \left(age_{\max} - age_{\min}\right) * \frac{x}{\alpha}$$

The figure below shows the resampling distributions for different values of R/L_f ,with the x-axis being normalised to $age_{\min} = 0$ and $age_{\max} = 1$. We can see as the fragment length gets longer relative to the radius, we will tend to sample older ages (that is the section of the grain that does not contain any part of the 2 terminations). If $R \geq L_f$ the sampling is set to be uniform (as in the first panel below).

Figure showing the distributions from which predicted ages are sampled for 0T grains when using forward models, with no input data constraints. The 4 panels are for different R/Lf ratios

Kinetic parameters for diffusion

For each grain you need to enter an activation energy (**Act Energy**), and diffusivity at infinite temperature (**Do**) and the helium ejection (**He ejection)** distance. These will be initially set to standard default values for apatite, with the Helium ejection distance being calculated (following more or less Ketcham et al, 2011) as a function of U, Th and Sm contents, if these are input In terms of the calculation, the input age should be the uncorrected (i.e. no FT correction) age, as the He-ejection effect is calculated as part of the thermal modelling. If you edit these default values (for example to simulate alpha ejection in zircon), they will not be recalculated.

If you want to use the corrected age, then set the helium ejection distance to zero. If the He ejection distance is not zero and you have input an age not equal to that calculated from the input U, Th and He, then the input age will be replaced by the calculated age. To avoid this set the He ejection distance to zero.

Finally, you can select from published **Radiation Damage Models** to allow for the possible effect of alpha damage on the diffusivity of He in apatite (Gautheron et al. 2009, Flowers et al. 2009, Willett et al. 2017 and the model discussed in Recanati et al. 2017) or zircon (Guenthner et al. 2013, Ginster et al 2019, Guenthner (2020)). The model described by Recanati et al. (2017) is identified as **G2015** in the dropdown menu.

To speed up the calculation of the radiation damage influence on diffusivity, QTQt takes advantage of the fact that the formulations for the Gautheron et al. (2009), Flowers et al. (2009) and Guenthner et al. (2013) can be linearised in terms of eU. Then the effective accumulated alpha damage (AAD) over time needs to be calculated for one grain with a reference value of eU (the first grain in the data file), and the results can be rescaled by the actual value of eU for the other grains. Note that the radiation damage effect is independent of grain size. The reference calculation needs to done for apatite and zircon, so it is a good idea to create a data file with all AHe data first then any ZHe data (or vice versa).

The Willett et al. (2017) and the Ginster et al (2019)/Guenthner (2020) use a different formulation to the other radiation damage models, and the full calculation is relatively slow, particularly when using several grains for a given sample. To speed up the calculation in these cases, QTQt can implement an interpolation based approach in which we do the full calculation for 4-5 grains (which must include the grain with the minimum and maximum values of eU and 2-3 other grains between these limits). The accumulated alpha damage (AAD) over time is stored for these grains and this is interpolated for the remaining grains. The conversion of AAD to diffusivity is relatively fast. An example of how to set up a data file (this needs to be done manually once a data filer has been created is given at the end of this section.

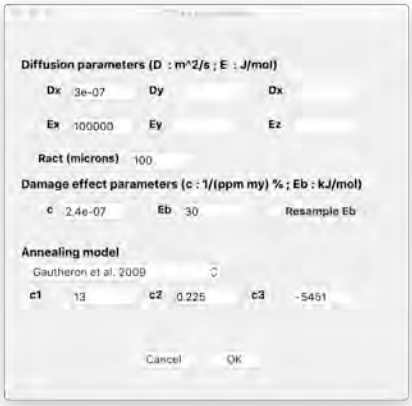
Note : in the current version of QTQt, you can not mix different radiation models in the same data file when using the interpolation approach mentioned above with either the Willet or Ginster models. In that case you need to put any additional He data (if you have AHe data, and/or are using a different radiation damage model for example) in different data files (you can use the same elevation in each file though). If you have not too many grains (< 6-8) with ZHe data, then you can probably use the full calculation (i.e. not bother with the interpolation approach).

Note radiation damage models will not be available if there are no U, Th and He concentration data enter for any analysis from a given sample. The U (and Th) ppm values are required if you want to use a radiation damage model for either apatite or zircon. If you input just U concentration, this will be used as the effective uranium (eU) value.

Note : if you choose a radiation damage model and input a value of 0 for eU (or U, Th) for the first sample in the data file, then the results (predicted ages) may be erroneous. To speed up the calculations, the first value of eU for data using a given radiation damage model is used as a normalisation value to recalculate the diffusivities for other samples with different values of eU. Using 0.0 is therefore not recommended. You can just use a small value of eU (e.g. 1ppm).

The kinetic parameters (**Do** and **Act Energy**) will be modified to show the published values for equivalent eU = 0 (for apatite) or α-dose = 10^{14} α/g (for zircon). according to the choice of radiation damage model and mineral selected. The calculation for He diffusion with radiation damage will always use the published values, even if you change them by editing the data file.

The model **G2015** requires some additional parameters, which can be specified in the dialog box that will appear if you select this option, as below



The model was initially set up to allow for anisotropic diffusion parameters, but this is not implemented in the current version of QTQt. The parameters considered by Recanati et al. (2017) are the damage effect parameters (c : ppm/my % and Eb : kJ/mol) and Eb can be sampled as an inversion parameter if desired, and then you need to define a maximum and minimum value (input boxes will appear if you select this option). It is also possible to modify the annealing model used for the radiation damage, using the drop down menu to select one of Gautheron et al. (2009), Ketcham et al, (2007), or Laslett et al. (1987). These use different values of the annealing model parameters, with defaults as follows :

Gautheron et al. (2009)	c1 = 13; c2 = 0.225 c3 = -5441	(radiation damage model = 4)
Ketcham et al. (2007)	c1 = 0.83 (= rmr0); c2 = 0.0 c3 = 0.0	(radiation damage model = 5)
Laslett et al. (2007)	c1 = -4.87; c2 = 0.000168 c3 = -28.12.	(radiation damage model = 6)

If no radiation damage model is selected, then the default kinetics for apatite are from Farley (2000) and for zircon from Reiners et al. (2004).

Given the uncertainty around the estimates of eU, it is possible to allow the input value to vary with a range defined as ± X%, for $0 < X \leq 100$. When you check the **Resample eU** checkbox, an text input box will appear as below.

Note : if you choose to vary eU this will override any choice you made to resample the He age, or rescale the age error for all samples in a run. This is partly for coding reasons, but also it is not a good idea to let too many parameters vary at the same time, as it then becomes more difficult to understand what is controlling the sampling and the final distributions on the thermal histories, predicted values, etc.

You can add another analysis for the same sample (**Add more**) and you can have up to 30 separate analyses for a given sample, and these can be different isotopic systems, with different input parameters.

As mentioned at the beginning of this section, you can input any single domain diffusion data (e.g. U-Pb ages from apatite). You just need to put in the ages, grain dimensions and the appropriate diffusion kinetics (**Do** and **Act Energy**). Set the alpha ejection distance to zero if appropriate (or select other as the mineral type).

The general He age data and parameters in the pre-version 5.4.1 data file would look as below, with the explanation in the right hand column. See appendix 1 for a description of the basic data file structure.

2	No of He ages
0	0 = No radiation damage, 1 = Gautheron, 2 = Flowers (-2 = Willett), 3-Guenthner (-3 = Ginster), and 4-6 are the Recanti models (and see last line in this table).
51326 23. 72.0 0.0 15.97 0.64 100.0 0.0 0.0	He, U, Th, Sm; Age, Error; length, width thickness
20.66 0.0032 138000.0	He ejection, Do, Act. Energy
2.4e-07 30 0.83 0.0 0.0	For the Recanti models there is an additional line for each sample with the values of c (ppm/my %) and Eb (kJ/mol) and the 3 annealing model parameters c1, c2 c3, if required. To the left is an example for the radiation damage model = 5.

Note the either age or error will be negative (not both) if you selected a resampling option for one of them (you can only choose one or the other for resampling). The negative sign indicates which value will be perturbed.

An example of the 5.4.1 data file would look as below, with the explanation in the right hand column and see the footnotes for the codes for Mineral ID and Crystal Geometry. Note in this case, you can mix different minerals, and use different radiation damage models or crystal geometry. The radiation damage parameter on the 2nd line will be ignored.
QTQt is backwards compatible with the earlier format.

6	No of He ages
0	0 = No radiation damage, 1 = Gautheron, 2 = Flowers, -2 = Willett, 3-Guenthner, -3 = Ginster, 4-6 Recanati models; 7 = mixed models (e.g. apatute and zircon in the same data file)

2.284E+10 8.570E+11 7.366E+11 0 17.21 0.860 81 0 0	He, U, Th, Sm; Age, Error; length, width thickness
A 19.46 6.0714e-5 122300 2 2 10	Mineral ID[1], He eject, Do, Act. Energy, Raddam model (codes as above), Crystal Geometry[2], eU/Rs sampling[3] Note : the the table above for the extra parameters required for the Recanati models.
2.284E+11 8.570E+12 7.366E+12 0 17.21 0.860 81 0 0	
A 19.46 6.0714e-5 122300 2 2 20	
5.954E+09 3.442E+11 4.037E+11 0 10.54 0.527 81 0 0	
A 19.62 2.0e-7 109200 1 2 0	
5.954E+10 3.442E+12 4.037E+12 0 10.54 0.527 81 0 0	
A 19.62 2.0e-7 109200 1 2 0	
2.93E+06 426.4 180.6 0 51.49 2.574 81 0 0	
Z 15.65 19.3188 165000 3 2 0	
2.93E+07 4264. 1806. 0 51.49 2.574 81 0 0	
Z 15.65 19.3188 165000 3 2 0	

Note : if you have chosen resampling for a given sample age, then there will be a minus sign in front of that age in the data file. Similarly, if you have chosen resampling for the error on a given age, there will be a minus sign on the error in the input file. You can not choose to resample both the age and the error.

Note : if you edit a data file subsequently and change the radiation damage model (from Flowers to Gautheron, for example) you only need to change the code for the Raddam model (from 2 to 1). The Do and E parameters will be automatically selected for the Raddam code when you read in the data file.

1 Mineral ID are given as Apatite = A, Zircon = Z, K-Ar/Ar = K, other = O

2 Crystal geometry 2 = sphere, 1,, infinite cylinder, 0 – infinite slab.

3 set to 0 for no sampling of eU value, or to a value <=100, as the ±% variation allowed on the input eU value. If you want to sample the effective spherical radius, set this value to -1 for random Monte Carlo sampling, and -2 for Markov Chain Monte Carlo sampling. This option is only possible for the mineral code Other and can not be used at the same time as resampling of eU, age or error.

Setting up data files for interpolation with the Willet and Ginster radiation damage models.

You can create a data file in QTQt and then you need to edit the file manually. As mention above with this interpolation option, you can only have ZHe or AHe data (not both) in a given data file.

In the data file, the default radiation damage flag for the Willet model is -2, and for the Ginster model it is -3.

An example of the part of a data file with AHe data, using the Willett radiation model is given below. The 19 is the number of grains and the -2 indicates the Willett radiation damage model.

19
-2
0. 10 0. 0.0 104.28 6.98 60.0 0. 0.0
A 20. 6.0 0.0714e-5 122300 -2 2 0
0. 20 0. 0.0 104.28 6.98 60.0 0. 0.0
A 20. 6.0 0.0714e-5 122300 -2 2 0
0. 30 0. 0.0 104.28 6.98 60.0 0. 0.0
A 20. 6.0 0.0714e-5 122300 -2 2 0
0. 40 0. 0.0 104.28 6.98 60.0 0. 0.0
A 20. 6.0 0.0714e-5 122300 -2 2 0
etc..

In this case, the full radiation damage will be run on every grain.

To use the interpolation approach we need to reorganise the data file so that we choose how many grains to do full calculation, and these need to be in the data file in order of increasing eU. The radiation damage flag is modified to indicate how may full calculation grains we use.
An example for the Willett model is below.

19
-24 - -2 = Willett, and the 4 indicates the first 4 grains will have the full calculation (-211 would imply first 11 grains)
0. 10 0. 0.0 104.28 6.98 60.0 0. 0.0 1st grain is the minimum eU
A 20. 6.0 0.0714e-5 122300 -2 2 0
0. 50 0. 0.0 104.28 6.98 60.0 0. 0.0 intermediate grains in order of increasing eU up to the max
A 20. 6.0 0.0714e-5 122300 -2 2 0
0. 110 0. 0.0 104.28 6.98 60.0 0. 0.0
A 20. 6.0 0.0714e-5 122300 -2 2 0
0. 160 0. 0.0 104.28 6.98 60.0 0. 0.0 4th (or 11th, etc) grain is the maximum eU
A 20. 6.0 0.0714e-5 122300 -2 2 0
0. 20 0. 0.0 104.28 6.98 60.0 0. 0.0 the rest of the grains can be in any order for eU
A 20. 6.0 0.0714e-5 122300 -2 2 0

U-Th zoning and Zoned crystals

If the crystal is zoned in U, Th or Sm, then you can input the zoning by clicking on the **Crystal Zonation** check box. Note that this option will not be accessible until you have put at least one of the crystal dimensions and will only be accessible for a spherical geometry. The zoning is defined in a spherical crystal (and the maximum radius will be defined by the equivalent radius for the crystal dimensions you have entered).

Clearly zoning influences the spatial distribution of He production within the crystal. If a radiation damage model has been selected, then the diffusivity will also change spatially as a function of the alpha-recoil damage effect (see Gautheron et al. 2009, Flowers et al. 2009). These two spatial effects are dealt with by using a finite difference method to calculate the distribution of He within the crystal. This numerical method is slower than that using for homogenous U, Th, and Sm distributions.

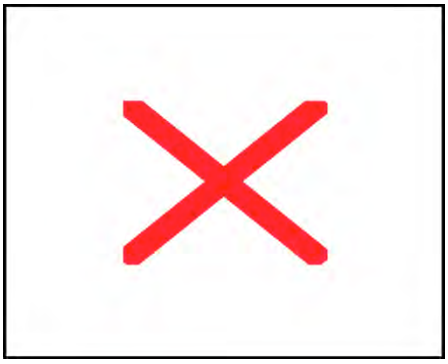
Having clicked on this check box, the window below will appear.

You will see the first two lines are filled in with the values from the general He input window. To enter new values click on the line below the last entry (line 3 in the example above). You will see the last line will move down and a blank line will appear above it. You need to input the R (radius) coordinate in increasing order and also input values (in ppm) for U, Th and Sm, even if they do not change at the input R values or are all zero. You need to use tab to move to the next cell in the table. You can input up to 20 discrete values, the first one being at R = 0, the centre of the crystal and the last one being the edge of the crystal (defined by the equivalent radius, written in red in this window).

If you have selected the **Constant between input values** (the default) option, you will see the last line will change to have the same concentration values as the previous line. This is due to the structure of the zoning as described below.

The structure of zoning can be specified in two ways, either as **Constant between input values** or I**nterpolate between input values**. For example, if we input the following data

R (microns)	U (ppm)
0	30
30	20
60	10
100	10



The 2 possible distributions are shown to the right. In red is the constant value between the nodes, in which the input concentration value is used from the input node value to the next node (note the last 2 nodes need to be the same value). In blue is shown the interpolated distribution in which interpolates linearly between adjacent nodes. For a linear concentration gradient from the centre to the edge, you would just need to put in 2 values, the first at the centre (R = 0) and the second at the edge (R = equivalent radius).
You chose between the 2 possibilities using the appropriate check box.

It is possible to try and estimate the structure of zoning using a similar MCMC approach to the thermal history modelling, although this is still in development (**so much so that I have pretty downgraded this option in the current version, but you need to input the number of iterations for the sampling of the zonation parameters**).
Given that the $^{4}He/^{3}He$ data are not too sensitive to different parent elements, it is a good idea to input the effective uranium (eU) for U concentration and set Th and Sm to zero. Then the estimation will be just on the combined parent (eU) rather than each element separately. This helps speed up the modelling.

The average of the concentration zoning is constrained to be constant (and equal to the input concentrations for the crystal). This is of use only for $^{4}He/^{3}He$ degassing spectrum data. It is possible to infer the number of zones (you need to define the minimum and maximum values allowed), and the locations of boundaries and the concentration for each zone. If the minimum and maximum number of zones are equal then it is just the locations and concentrations that are inferred for that number of zones. It is also possible to vary just the concentrations or just the zone boundaries (although in both cases the constraint that the average of the zoned concentration is constant is imposed), or fix the zoning to the input distributions (so no inversion is done for the zoning).
The final parameter to specify is the number of iterations for the zoning (see the example file below).
The inversion process involves the inference of zoning and the thermal history. Consequently it becomes fairly slow.

Notes on zonation data
1. If the input distribuution has a maximum value either greater or less than the equivalent radius, QTQt will adjust the distribution to have the equivalent radius as the maximum by either deleting or adding points as required, and using the concentration of the adjacent node.

2. QTQt will calculated the average U, Th and Sm distributions for the zonation and update the values in the standard U-Th/He data window (and the output data file).

3. At the moment, QTQt allows only the first crystal in a given sample to have zoning. This can be a crystal with or without $^{4}He/^{3}He$ data. If you want more than one crystal from the same sample to have zoning, you can just treat them as separate samples (and model a vertical profile with a small difference, e.g. 0.1 m, in the elevation of each sample).
The general He age data with zoning are illustrated below.

The difference to non-zoned data files is that the zonation information is added in before the alpha ejection, and kinetic parameter line.

2	No of He ages
0	0 = No radiation damage, 1 = Gautheron, 2 = Flowers, etc..
51326 -23. -72.0 -0.0 15.97 0.64 100.0 0.0 0.0	He, U, Th, Sm; Age, Error; length, width thickness
4	Number of zones (negative value if interpolation to be used)
0.0 40. 70. 0.	R, U, Th. Sm
30.0 30. 80. 0.	
70.0 20. 80. 0.	
100. 20. 80. 0.	
1 1 5 100	Code for zoning inversion, minimum and maximum number of zones (set these to the same value to fix the number of zones to a constant), number of iterations for MCMC sampling of zonation
20.66 0.0032 138000.0	He ejection, Do, Act. Energy
0.0 0.0 0.0 0.0 29.0 -0.5 100. 0.0 0.0	
20.0 0.0032 138000.0	

Note the standard input U, Th and Sm values (in the 3rd line for example) will now have a minus sign in front to flag that we have zoning. You need just one of these to have the minus sign for zoning to be activated.

Also, the input number of zones can be positive (for constant values between nodes) or negative (for interpolation between nodes).

The codes for the zoning inversion are
0 : invert for number of zones, the boundaries and the concentrations.
1 : invert for the boundaries and the concentrations (number of zones fixed).
2 : invert for the boundaries only (although concentrations will be adjusted to satisfy the constant average concentration constraint).
3 : invert for the concentrations only (boundaries fixed)
4 : invert for the number of zones (although boundaries can vary and concentrations will be adjusted to satisfy the constant average concentration constraint)
5 : Fix the zoning to the input values (no inversion for zoning).

^{4}He/^{3}He data

To include such data in the modelling process, you need to have the data in a separate file, in the following formats (provided by Ryan McKeown and David Shuster at University of California at Berkeley).

```
% grain_radius(cm)  grain_radius(cm) bulk[U](ppm) bulk[Th](ppm) age1 delage1 minimum and maximum weighting
0.00701 0.00701 18.2 0.00 142.7 43.9 0.1 1.0
% Step   3He ((10^6 atoms) ±  Rs ±
1          0.4036    0.0190    54.3      48.3
2          0.3667    0.0180    202.2     55.1
3          0.6296    0.0244    346.4     34.7
4          1.4164    0.0376    552.4     20.4
5          0.7489    0.0268    677.7     37.8
6          0.7338    0.0265    712.0     39.6
7          0.7815    0.0274    882.4     42.6
8          0.7072    0.0260    1128.0    53.2
9          0.6365    0.0245    1378.6    67.1
10         0.5345    0.0223    679.83    50.5
12         0.6623    0.0251    1841.9    82.3
13         0.8502    0.0287    2519.5    91.8
14         0.7371    0.0266    2954.8    116.6
15         0.7712    0.0272    3408.4    129.3
16         1.2202    0.0348    3501.5    100.5
17         1.8336    0.0430    3821.5    86.3
18         1.7347    0.0418    4078.1    94.5
19         1.8117    0.0428    4385.9    99.3
20         0.0595    0.0054    5834.8    1604.9
21         0.0146    0.0016    1422.6    1977.1
22         0.0178    0.0019    1076.0    1420.3
```

Note that the radius in input twice. This is for historical reasons. Currently, the details of the radius, concentrations, and age in this data file should be the same as those for the first He sample in your standard QTQt data file.

It is also possible to input the ^{4}He/^{3}He data as the cumulative ^{3}He loss (F^3He) and R_s/R_{bulk} as shown below.

```
% grain_radius(cm)  grain_radius(cm) bulk[U](ppm) bulk[Th](ppm) age1 delage1 minimim and maximum weighting
0.00701 0.00701 18.2 0.00 142.7 43.9 0.1 1.0
% Step  F3He  +/- Rs/Rbulk +/-  errors
1          0.024     0.024     0.023     0.020
2          0.046     0.046     0.085     0.023
3          0.084     0.084     0.146     0.015
4          0.169     0.169     0.232     0.009
5          0.214     0.214     0.285     0.016
6          0.258     0.258     0.299     0.017
7          0.305     0.305     0.371     0.018
8          0.347     0.347     0.474     0.022
9          0.385     0.385     0.579     0.028
10         0.417     0.417     0.286     0.021
12         0.457     0.457     0.774     0.035
13         0.508     0.508     1.058     0.039
14         0.552     0.552     1.241     0.049
15         0.599     0.599     1.432     0.054
16         0.672     0.672     1.471     0.042
17         0.782     0.782     1.605     0.036
18         0.886     0.886     1.713     0.040
19         0.994     0.994     1.842     0.042
20         0.998     0.998     2.451     0.674
21         0.999     0.999     0.598     0.831
22         1.000     1.000     0.452     0.597
```

Finally QTQt can handle a combination of the two input formats (e.g. F^3He and R_s, ^3He atoms and R_s/R_{bulk}). It tests for F^3He by checking that the last value in the 2nd column is the largest and is equal to 1.0 and for R_s/R_{bulk} by checking that largest value in the 4th column in < 10.

If there are steps that are considered unreliable, you can make the step index (the first column) a negative value, and these steps will be ignored in the modelling process, but these values will be plotted on the output spectrum (indicated by red bars for such steps).

The weighting parameters (the last 2 values in the first line) allow you to vary the influence of the $^4He/^3He$ data relative to other data (e.g. AHe ages or AFT data) when estimating the thermal history. In essence, the errors on each step are multiplied by the weighting factor, so a value < 1 will increase the influence of the $^4He/^3He$ data and a value > 1 will reduce the influence. If you set both values to the same value, then the weighting will be constant (at that value). If you input 2 different values, then QTQt will sample the weighting value between the 2 input values.

The name of the $^4He/^3He$ data file must be the same as the general data file, with 43 added at the end, before any ".". For example, if the general data file (with AFT and AHe data for example) is called "Mydata.txt", then the name of the $^4He/^3He$ data file needs to be "Mydata43.txt". This file must be in the same directory as the general data file.

Once you have run a thermal history model (forward or inverse), you can look at the results using the plotting options described later. To look at the $^4He/^3He$ spectrum for a given sample rather than the default fission track and/or total grain helium ages, just hit the command or shift key on a Mac, or the control or shift key on a PC. To return to the default, hit the control or option key on a Mac or the alt key on PC.

If you have only $^4He/^3He$ and standard He ages, the plot will always be of the spectrum.

Note : when you enter $^4He/^3He$, QTQt will calculate the diffusivity for each heating step to produce the equivalent 3He loss. This can be a little slow, so to reassure you, a dialog window will appear, as below..

Just click on OK then wait (a minute or so)...

$^{40}Ar/^{39}Ar$ data

To include such data in the modelling process, you need to have the data in a separate file, in the following format (modified from a format provided by Peter Zeitler at Leigh University). The modelling uses the MDD approach, and Peter Zeitler provided the calculation routines (based on the publications and code of Oscar Lovera, University of California Los Angeles).

```
0.00000000000001                    Convergence criterion for series sum
1                                   Geometry flag  : 1 = sphere, 2  = slab.
6                                   Number of domains
33.12 6.3010 0.16667                Act. energy (kcal/mol=4.184 kJ/mol), log10(Do/a2), propn of domain
33.12 5.6990 0.16667
33.12 5.3468 0.16667
33.12 5.0969 0.16667
33.12 4.9031 0.16667
33.12 4.7447 0.16667
20                                      Number of heating steps.
0.08040 27.243   1.0000   1   Fraction released, age (Ma), Error on age (Ma) 1 (0)–use  for fitting (or not)
0.11170 45.861   1.0000   1
0.13260 53.636   1.0000   1
0.14550 58.686   1.0000   1
0.15470 62.478   1.0000   1
0.16700 65.519   1.0000   1
0.17790 68.064   1.0000   1
0.18950 70.321   1.0000   1
0.20140 72.489   1.0000   1
0.22590 74.760   1.0000   1
0.25270 77.172   1.0000   1
0.26820 79.549   1.0000   1
0.28340 81.719   1.0000   1
0.30450 83.621   1.0000   1
0.32790 85.403   1.0000   1
0.37820 87.227   1.0000   1
0.56170 89.106   1.0000   1
0.63300 90.944   1.0000   1
0.81650 92.713   1.0000   1
1.0000   94.657   1.0000   1
```

The name of the $^{40}Ar/^{39}Ar$ data file must be the same as the general data file, with Ar added at the end, before any ".". For example, if the general data file (with AFT and AHE data for example) is called "Mydata.txt", then the name of the $^{40}Ar/^{39}Ar$ data file needs to be "MydataAr.txt". This file must be in the same directory as the general data file.
If the number in the last column is > 0, then this step will be used in the inversion data fitting process. If you decide you do not want to use a step, just set this to a negative (or zero) value.

Once you have run a thermal history model (forward or inverse), you can look at the results using the plotting options described later. To look at the $^{40}Ar/^{39}Ar$ spectrum for a given sample rather than the default fission track and/or total grain helium ages, just hit the command or shift key on a Mac, or the control or shift key on a PC. To return to the default, hit the control or option key on a Mac or the alt key on PC.

Single crystal age profile data

If you have age profile data across a single crystal, you can input that in the following way. You need to create a generic QTQt data file as described above (let us call it "Mydata.txt",), and add in 1 He (or equivalent age). So at the end of the data file we would have something as below...for a crystal with an (U-Pb) age of 1960 Ma and error of 40, with a spherical grain of radius 144 microns...

1
0
0 0. 0 0 1960. 40. 144. 0 0
A 0. 1.27e-8 228500. 0 2

Here, for the final line, the A means apatite, the next 0. means no ejection correction, the next 2 values are Do and E for this diffusion system and the next 0 before the 2 means no radiation damage model, and the final number 2 means spherical geometry. See the section on inputting He data for a full description of the possible values of these parameters for other mineral/isotope systems ans crystal geometries.

Then, similar to the input for $^{4}He/^{3}He$ and $^{40}Ar/^{39}Ar$ data, we have an additional file, with the same name, but adding Pr prior to any '.txt' string. So if we have "Mydata.txt" as the generic QTQt datafile , we need a file called "MydataPr.txt", with the structure described below. You can enter the coordinates of the spot ages as either the radius (distance relative to the centre) or as the distance relative to one edge. For the first option, we enter the radius on line 2 of this file, and for the second option, we enter the diameter (and put a minus sign in front to flag it is the diameter).

%Dummy line	
-288.	Crystal radius (microns) or diameter (which is flagged with a minus sign)
11 1.0	No. of ages, error weighting
%Dummy line	
1 1725. 44. 0.425 0.012 0.1627 0.0052 13.1	Index, age, error, C1, eC1, C2, eC2, Coordinate
2 1752. 20. 0.559 0.011 0.2834 0.0069 39.3	
3 1864. 25. 0.4038 0.0082 0.203 0.0047 65.5	
4 1855. 27. 0.3834 0.0081 0.1979 0.0044 91.6	
5 1895. 29. 0.3798 0.0072 0.2075 0.0049 117.8	
6 1902. 27. 0.3766 0.0077 0.2031 0.0049 144.0	
7 1960. 28. 0.3736 0.008 0.204 0.005 170.2	
8 1903. 33. 0.367 0.0075 0.1983 0.0056 196.4	
9 1955. 31. 0.3539 0.0064 0.19 0.0045 222.6	
10 1877. 29. 0.3776 0.0072 0.1978 0.0045 248.7	
11 1811. 28. 0.4017 0.0082 0.2088 0.0047 274.9	

Here index is an integer identifier of the data point
The age and error are obvious..
C1 is a concentration measure (e.g. U/Ca for U-Pb dating) which would be used to allow for zoning in the parent isotope, and so in the production of the daughter
eC1 is the error in this concentration measure;
C2 and eC2 are similar concentration measures, but are not used currently.

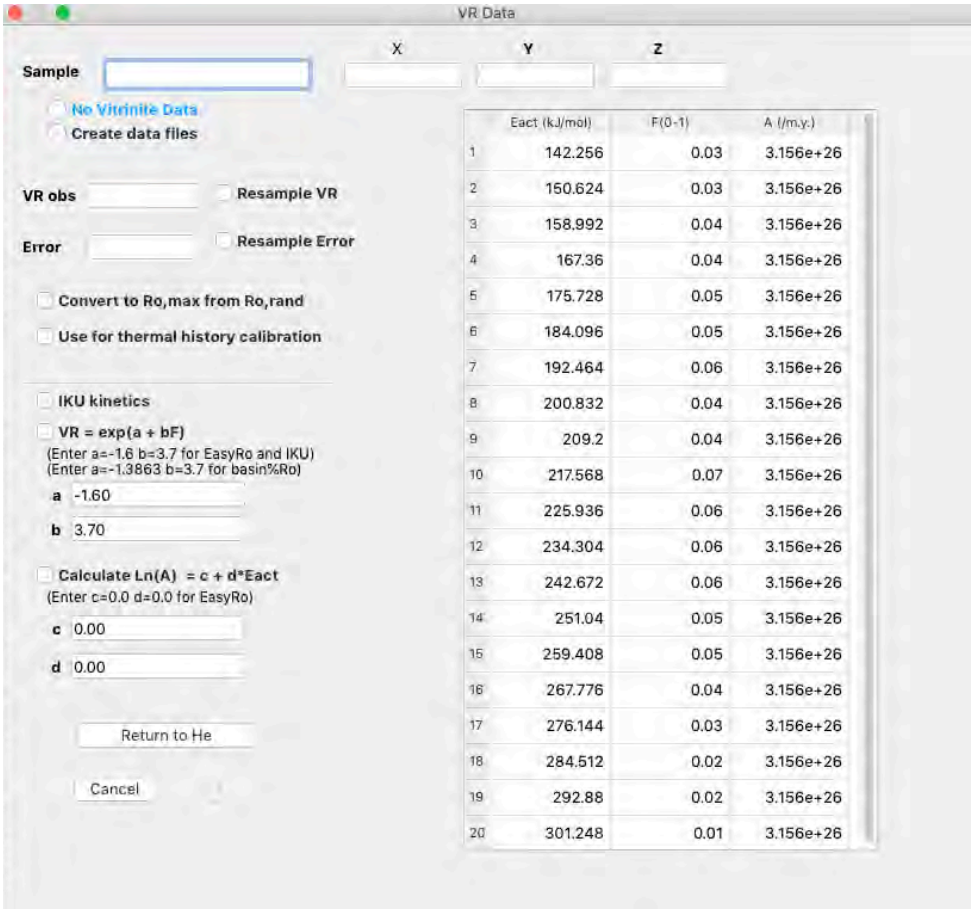
Coordinate is the either the radius (distance from the centre) or the distance from one side of the crystal to the measurement position (so the maximum measurement will be the diameter). In the example above the diameter of the crystal is 288 microns (or radius of 144 in the generic QTQt file), and the coordinates of the age profile go from 13.1 microns to 274.9 microns from (almost) one edge to the opposite side of the crystal. QTQt will convert the diameter coordinates to radius. The coordinate data can be input in any order as QTQt will sort the input based on the radius.

The concentration profile is interpolated (linearly) and normalised to the maximum value. The production of the daughter is scaled according to this concentration distribution. If you are not worried about spatial variations in production, just set the concentration to 1.0 everywhere.

To see the model results choose the plot option **Plot Individual Predictions** (the plotting options are described in more detail later).

Vitrinite Reflectance data

Once you click on **OK**, the following window will appear to allow the input of vitrinite reflectance.



If you have no VR data, lick on **No Vitrinite Data**. Otherwise, you can enter a (mean) observed vitrinite reflectance (**VR obs**), with an error value, (**Error**) as well selecting whether or not to use the observed value as a constraint (**Use for thermal history calibration**) for the inverse modelling (if not, then you can still plot the predicted vitrinite reflectance for various thermal history models once the inversion run has finished). The table on the right shows the default kinetic parameters, for Easy%Ro (from Sweeney and Burnham,1990). You can enter up to 20 of your own values (Eact = Activation Energy, F is the stoichiometric factors, which need to total 1, and A is the frequency or pre-exponential, factor which may or may not be constant).

Alternatively, there is the option to create a series of vitrinite reflectance only data files, using the button **Create data files**. This is useful for well data and requires an input text file in the format given in the table on the next page. The input data include stratigraphic information (depth to top of a stratigraphic layer and the age, including a depth and age for the bottom of the well), downhole temperature data (at least the surface temperature and one other temperature measurement is required) and measured vitrinite reflectance at different depth.

Note : the maximum depth in the stratigraphic information must be at least as deep as the deepest vitrinite reflectance measurement. This is because the equivalent stratigrphic age at the depth of each vitrinite reflectance measurement is estimated by interpolating the input stratigrapic ages above and below the measurement depth.

From this input text file, a QTQt data file is created for each measured vitrinite reflectance value, using the name of the input text file, with the addition of the character string '_VR_XX.txt' where XX is a number from 0 to N-1 (N being the number of vitrinite reflectance measurements). These files will be in the same directory as the input text file.
The equivalent stratigraphic age and present day temperature values at the depth for each vitrinite reflectance measurement are interpolated from the input stratigraphic ages and temperature values. If the deepest temperature measurement is not as deep as the some of the depths for the vitrinite measurements, then the gradient between the 2 deepest temperature measurements is extrapolated.

Example of the input text file format required to create a series of QTQt datafiles for a series of vitrinite reflectance measurements in a well.

0.0	0.1		X and Y co-ordinates
7			Number of stratigraphic layers
0	7.5		Depth to Top and stratigraphic age
1432.	25		...
1572.	52.		...
2025.	65		...
2221.	78		...
2830.	119.0		...
4023.	124.0		...
3			Number of temperature measurements
0.0	12.0	5.0	Depth, Temperature (°C) and error on Temperature (°C)
2100.	70	5.0	...
4020.	118.	5.0	...
11			Number of vitrinite reflectance measurements
570.	0.23	0.02	Depth, Ro%, error on Ro%
900.	0.25	0.003	...
1121.	0.30	0.03	...
1348.	0.27	0.02	...
1517.	0.29	0.03	...
1739.	0.28	0.04	...
1913.	0.31	0.03	...
2315.0	0.33	0.03	...
2825.1	0.36	0.04	...
3305.0	0.40	0.04	...
3638.1	0.48	0.04	...
4020.0	0.54	0.03	...

Similar to the He age data description above, you can choose to **Resample VR**, which will sample the observed vitrinite reflectance from a normal distribution centred on the input value, with a standard deviation equal to the input error value. Alternatively, you can select **Resample Error**. This option samples a scaling factor for the input error, which is used in the calculation of the data fit. The scaling factor is between 0.1 and 10 so the data can effectively be treated as being more precise (low scaling factor) or less precise (high scaling factor), relative to the input error value. This may be useful when you are not sure of how good you error estimates are.
Note in the data file, the input value will be negative if you choose to **Resample VR** or the error will be negative if you choose **Resample Error**

You can input the data as $R_{o,rand}$, rather than $R_{o,max}$, and then convert to $R_{o,max}$, following Zhang and Davis (1993) using the check box **Convert to Ro,max from Ro,rand**.

There is a conversion of the calculated time-temperature integral to equivalent VR (**VR = exp(a + bF**), and again the default values for **a** and **b** are for Easy%Ro.

(NOTE As indicated in the dialog window you can modify the value for **a**, to use the basin%Ro model, calibrated by Soren Nielsen, Aarhus University and the model is described Nielsen et al. 2015) . If you enter a value of -1.3863, you will notice that the values of F (the proportion of each reaction with a given activation energy) will change to the values proposed by Nielsen et al. (2015). Resetting this to -1.6 will reset these values to the original Easy%Ro.

To use the kinetics for the IKU model of Ritter et al. (1996), check **IKY kinetics**. This model uses the same conversion factor as Easy%Ro.

Finally, you can also enter a function (**Calculate Ln(A) = c + d*Eact**) to calculate the frequency factor (A) as a function of the activation energy (Eact). This needs to be a log linear relationship and the default parameters (**c** = **d** = 0.0)are equivalent to EasyRo.

If you choose to create the vitrinite data files using the button **Create data files**, these will all have the values of the other parameters (e.g. **Resample VR**, the kinetic parameters and the VR calibration values) that are in the vitrinite dialog window at the time you select **Create data files**.

In a QTQt data file, the vitrinite reflectance data and parameters typically look as below

-1	No. of VR observations **(usually one but this needs to be negative as a flag to indicate VR data)**
0.833180 0.200000	VR obs, VR error (one can be negative if resampling has been selected)
1	1 (or 0) indicates used as a constraint (or not)
-1.3 3.7 0 0	Conversion to VR parameters (**a,b,c,d**)
20	No. of activation energy values
142.256 0.030000 3.1536e+26	Act Energy, Proportion, Frequency factor
150.624 0.030000 3.1536e+26	
158.992 0.040000 3.1536e+26	
167.360 0.040000 3.1536e+26	
175.728 0.050000 3.1536e+26	
184.096 0.050000 3.1536e+26	
192.464 0.060000 3.1536e+26	
200.832 0.040000 3.1536e+26	
209.200 0.040000 3.1536e+26	
217.568 0.070000 3.1536e+26	
225.936 0.060000 3.1536e+26	
234.304 0.060000 3.1536e+26	
242.672 0.060000 3.1536e+26	
251.040 0.050000 3.1536e+26	
259.408 0.050000 3.1536e+26	
267.776 0.040000 3.1536e+26	
276.144 0.030000 3.1536e+26	
284.512 0.020000 3.1536e+26	
292.880 0.020000 3.1536e+26	
301.248 0.010000 3.1536e+26	

IMPORTANT – when you have input vitrinite reflectance data, QTQt will assume that this is a sediment. Then you will need to input a time-temperature point (or box) as constraints for the stratigraphic age, and also some constraint on the present day temperature. This is described in the next section.

Once you have entered the data, a final window will appear will provides a short summary and allows to you to choose certain modelling parameters (e.g. the annealing model for fission tracks).

Note : when you want to save the input data, you should click on the button  However, if you hit OK, you will also be prompted to save the file.

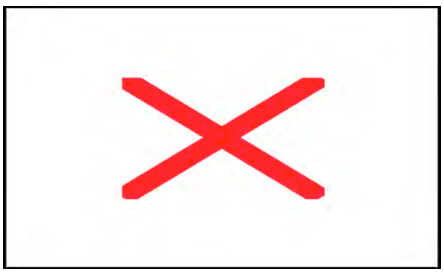
Required parameters are missing or incorrect.

This window allows you to set the fission track annealing and compositional models, as well as sample specific thermal history information for the current sample (data file) being created. The **Constrained point** option is intended to be used with sedimentary samples for which you know the stratigraphic age and temperature at the time of deposition (these can be input as a range). If this option is selected, then you can select to allow for the possibility of a sample having preserved some record of the pre-depositional thermal history (**Allow for pre-depositional thermal history**) . If you select this, then another time-temperature point is used in the modelling, older than the stratigraphic age, to allow for the pre-depositional thermal history. It is assumed that the temperature of this pre-depositional point is within the range specified for general prior of the total profile (see the next section for discussion of this) and the time is between the stratigraphic age and the maximum time specified for the general profile. Even if the post-depositional thermal history implies that the sample is totally annealed/degassed, this pre-depositional time-temperature point can still be incorporated (it is not a significant computational overhead).

If you choose **Allow for pre-depositional thermal history**, then any time-temperature points sampled prior to the stratigraphic age will not be incorporated into the thermal history (apart from the one sampled pre-depositional time-temperature point). This applies to any hard constraints defined in the general thermal history prior. If you do not select **Allow for pre-depositional thermal history**, then it is possible to allow for one (older than stratigraphic age) hard constraint defined the general prior. For multiple samples, this point will be the same for all samples (unlike the sampled pre-

depositional time-temperature point). When calculating vitrinite reflectance, all pre-depositional time-temperature points are ignored.

This stratigraphic age and present day temperature constraints are required for any sample with vitrinite reflectance, and it is only the post-depositional thermal history that is used for modelling the vitrinite reflectance value for a given sample. If you have input vitrinite reflectance, you will see the window to the left as a reminder. Just click on OK to continue the input.



The **Constrained Present day** option can be used to set the present day temperature to be within given limits (mean±range) for any sample. This is most likely to arise for well data. If the **±Range** parameter is set to zero, the value will be fixed at the **Mean** value.

Note that if you set the present day temperature or stratigraphic age for one sample in a borehole or vertical profile, you need to set these parameters for all samples.

You can set the **Annealing Model** for a particular run using the dropdown menu. For the two Ketcham et al. models, you will need to set the **Compositional Model** parameter. **Value** is required according to the type of kinetic parameter you want to use. If you set the **Uncertainty** to 0, then the annealing model is chosen using this fixed value of the kinetic parameter. If you set the **Uncertainty** to a non zero value, then the compositional parameter is sampled from a normal distribution, with a mean equal to **Value** and a standard deviation equal to **Uncertainty**. This is one way to allow for uncertainty in the annealing models or their calibration.

You can set the Initial track length to a specified value. Note that for the Ketcham et al. annealing models, the default is to **Calculate initial track length** using the compositional information. You can uncheck this option if you do not want to do this.

The **Resample l/l0** option allows you to resample the initial track length ratio. This may be desirable not only because different analysts measure lengths differently, but also because the annealing experiments are based on laboratory timescales which may not capture low temperature annealing over geological timescales. For the Ketcham et al. (1999, 2007) annealing models, the default value is 0.893 (based on measurements made by Raymond Donelick), while for the Laslett et al. (1987) model the default is about 0.92. Using the resampling the l/l0 ratio can be varied between 0.8 and 1.0. During a particular run, the same resampled value will be used at a given iteration for all data sets that have this resampling option selected.

You can modify the annealing models parameters for **Use Projected lengths**, **Cf tracks**, or **Etchant** if desired, and the appropriate adjustment will be made to the annealing model predictions. Note if you use the Laslett et al. (1987) the options for Cf tracks, projected lengths, etchant, and the compositional parameters will not be used. The same applies to the 3 zircon models (and for these the appropriate default value for the initial track length will be inserted).

If the sample has He analyses, then the number of ages is summarised, together with the choice of alpha radiation damage model (one of : none, Gautheron, Flowers, Willett, Guenthner, G2016, or

mixed). Note this will be set to none if there are no U, Th and He concentration data enter for any analysis from a given sample as the U and Th concentrations are required for the alpha radiation damage models .

Finally, if you are building a QTQt file for the first time, or modifying an existing file, you can **Save data for reload**, and you will be prompted for a file name. If you do not select this, the changes will not be saved.

It is recommended to build all the data files you might need (for example samples from a vertical profile or borehole suite) and save them as you build them. When you want to proceed to running thermal histories models, it is probably best to quit QTQt and restart it.

Review existing QTQt data file

This allows you to open an existing data file and check or edit the values. This process follows the same progression as described above for creating a new QTQt data file. If you make changes to an existing datafile, you need to save them explicitly using the save data for reload in the final window as described above.

Input and modelling of detrital data

Following the article of Gallagher and Parra (2019), it is possible to model thermal histories from detrital data (from recent sediments representing a sample of a single catchment). The minimum data inout will be a detrital data set, and the present day distribution of the elevation in the catchment, i.e. the hypsometry. As shown in Gallagher and Parra (2019), it is possible to combine the detrital data with in situ or bedrock data (from a vertical profile for example). Note for the elevation in the detrital data file, you should use a value lower than the lowest elevation value in the catchment (which should be captured in the hypsometry data files).

The detrital data are in the same format as a general QTQt input file, but the data types are limited to apatite fission track and the 4 diffusion data types (apatite and zircon (U-Th)/He, K-Ar, and another, e.g. U-Pb in apatite). The different types of diffusion data are identified in the data files by the uppercase letters, A, Z, K and O.

Given the dependence of fission track annealing on compositional parameters, it is recommended to input groups of compositional ranges (see ***Compositionally binned count and length data***), as these will be used for the predictions of the detrital data.

For AHe/ZHe data, we can allow for different grain sizes, but the current version of QTQt does not allow for different eU values . Consequently, it is recommended you do not use radiation damage models, or if you do, then you can use just one value of eU for all AHe/ZHe ages. For the detrital data file the appropriate choice of radiation damage model should be defined for each grain as the option to specify a global radiation damage model (see appendix 1) is reserved (to allow for sport LA-ICP-MS ages …see below).

If the detrital age diffusion type data are LA-ICP-MS spot measurements you can opt to compare the measured age to that predicted in the centre of the crystal (the model crystal which will be a sphere, cylinder or slab) rather than the predicted whole grain age. You do this by setting the global radiation damage model parameter to -1 in the detrital data file. This parameter is the line after the total number of diffusion data grains (see Appendix 1).

For the diffusion-based detrital data as mentioned above, you can choose to not use the input data of given types for the inverse modeling. You do this by setting the appropriate uppercase letter (A, Z, K and O) to lowercase. This allows you to still make predictions and make a visual comparison to the observed distributions for those data.

The hypsometric data need to be in a file that has the same name as the detrital data, with 'Hy" added at the end of the name, but before an extension (e.g. txt). For example, if the detrital data file name is 'DetritalS.txt', then the hypsometry file needs to be called 'DetritalSHy.txt'. When you open a data file, QTQt will look to see if there is an equivalent hypsometry file in the same directory. If it finds one, then it decides we are using detrital data.

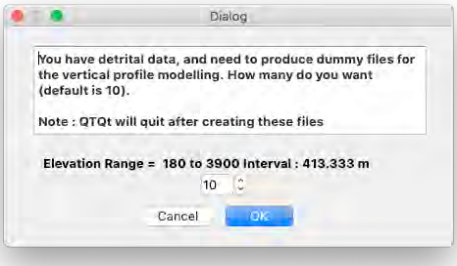
An annotated example of an input hypsometric curve is given below. The first line defines some parameters, followed by 2 columns with cumulative probability and elevation (in m).

11 0 D		**1st value :** No. of points in hypsometric curve **2nd value :** 0 = do not resample input TSF, 1 = resample input TSF with max likelihood estimate each iteration, 2 = resample TSF each iteration (using estimate from the previous iteration as the starting model) **3rd value :** D = model just detrital data, P = model just vertical bedrock profile data, A = model both detrital and vertical bedrock profile data together. ***Note if you have only detrital data the 3rd value should always be D.***
0.00	180.00	**1st value** = cumulative prob., **2nd value** = elevation (in order low to high)
0.10	614.00	
0.20	1015.00	
0.30	1241.00	
0.40	1503.00	
0.50	1826.00	
0.60	2060.00	
0.70	2229.00	
0.80	2449.00	
0.90	2850.00	
1.00	3900.00	

The method is based on predicting a vertical profile (e.g. AFT ages, track length distribution and AHe ages) in a catchment for a given thermal history. This is then sampled according to the Topographic Sampling Function (TSF), which is effectively a series of values between 0 and 1 used to weight the predictions from each elevation (as defined in the TSF) to produce a predicted detrital distribution. By default the TSF is equivalent to the input hypsometric curve, but this can be varied as part of the inversion. Currently, this is done by using iterative non-negative least squares to estimate the optimal (in the least squares sense) TSF for a given thermal history to produce a predicted detrital distribution that best fits the equivalent observed detrital distribution (e.g. for AFT ages). An alternative approach is to use MCMC sampling to produce a distribution of TSF for a given thermal history. This is not implemented in current version of QTQt (as it is considerably slower to run). As noted in the input hypsometry data file above, we can set a flag to fix the TSF equivalent to the input hypsometric curve, to use the input hypsometric curve as the starting TSF model at each iteration of the MCMC sampling for thermal histories, or to use the estimated TSF from the previous iteration as the starting model. Currently, I suggest it is probably better to use the TSF at each iteration, as some preliminary tests implied that we probably get stuck when we use the optimal estimate of the TSF from a previous iteration as the starting model for the next thermal history iteration.

The predicted detrital distributions are obtained by sampling, for example, AHe age elevation profiles predicted for a suite of dummy samples at elevations defined by the user. These elevations do not need to correspond to the values in the input hypsometric curve, but do need to have the same maximum and minimum elevations (as the hypsometric curve). QTQt can generate these dummy files automatically or you could create them by hand. Once you have created a detrital data file and

hypsometry data file for QTQt, you can open the detrital data file (and QTQt will look for the associated hypsometry file). Then, provided QTQt recognizes this is a detrital data file, you will see a dialog window as below :



This prompts you to select how many dummy files you want (default = 10) at equal elevation intervals between (and including) the minimum and maximum values found in the hypsometry file. The more files you choose, the slower QTQt will run as it needs to do a forward calculation for each dummy data file. As mentioned above, the elevations of these dummy files do not need to correspond to the values in the hypsometry file. The dummy files are used to predict a vertical profile (e.g. for AHe age for a given grain radius, or AFT age for a given compositional parameter) at the equivalent elevations in the dummy data files. The values for the elevations relevant to the TSF are obtained by interpolation.

Once the dummy files are created QTQt will quit.

If you have just a file with detrital thermochrometric data, and no in situ, or bedrock, data files, QTQt will also create 2 additional files corresponding to the lowest and highest elevations in the hysometry file. These will not have the word 'Dummy' in their titles, but will have either '_TOP' or '_BASE' at the end of the name, corresponding to the highest and lowest elevations in the hypsometry file. These should be opened when you open the detrital and other dummy data . The data in these 2 files will not be used in the modelling but they allow us to define the temperature offset/gradient parameters for the vertical profile modelling.

Again once these files are created QTQt will quit.

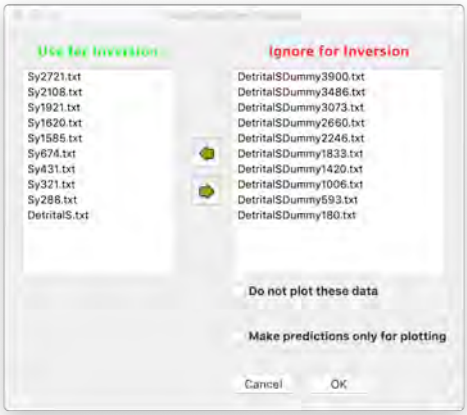
Note creating these files means you have only detrital data (i.e. no real in-situ vertical profile data)/ In this case, the 3rd value on the first line of the hypsometry input file should always be D (see above).

The dummy files need to have the word 'Dummy' (the case does not matter) in their name to allow QTQt to recognize they are not real data files. The data in the dummy files will be of a similar form to that in the detrital data file. They will have the same range of compositional groups and number of single grain ages and length measurements for AFT. For AHe/ZHe data, there will not be the same number of single grains as the actual detrital data, but QTQt will identify the maximum and minimum equivalent grain radii. It will uses these 2 values and 4 values at regular spacing between them to produce equivalent data for 6 values of the grain equivalent radius. Predictions will be made for AHe/ZHe ages with these 6 grain sizes, and the predicted ages are then interpolated to the appropriate equivalent grain radius for the measured/observed AHe/ZHe ages.

A similar approach will be implemented to allow for eU variations as well as grain size, requiring more input dummy grains and interpolation in 2D (eU and radius).

Once you have created the dummy files, you then need to open all the files, the detrital data file, the dummy files, and any real in situ/bedrock sample data files (or the 2 data files mentioned above, with '_TOP' or '_BASE' in the title). You do not need to open the hypsometry file. When you open these files, you will see a dialog window as below (for the case with no in situ or bedrock data).

You can see the two files with '_TOP' and '_BASE' in their titles in the left hand panel. As mentioned above, these allow us to define the temperature offset/gradient parameters for the vertical profile modelling. If we had opened some data files containing in situ/bedrock data from a vertical profile, the dialog window would look something like the image below,



These images highlight the fact that the dummy files (whose names include the word 'Dummy') are not used in the inversion.

After you have opened the appropriate data files, you will also see a summary statement in the main window of QTQt, as below

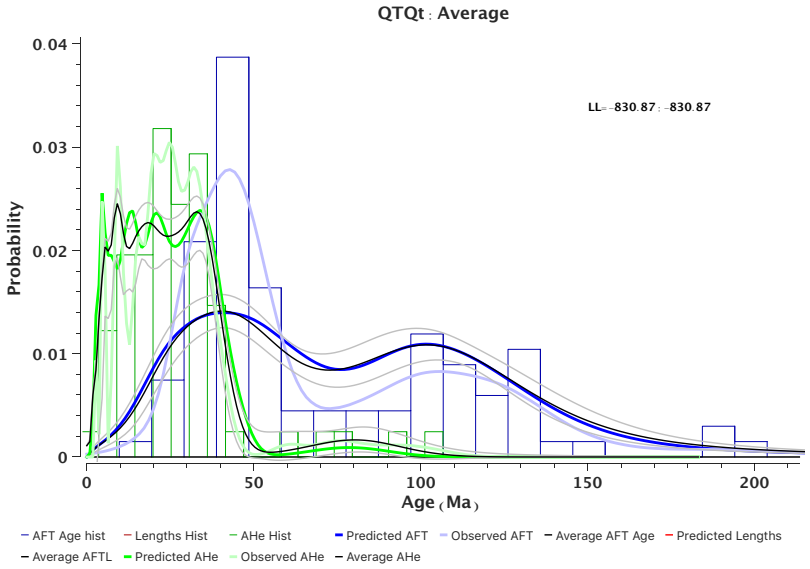
This summaries the input (that we have detrital data, only detrital data are being used in the inverse modelling and we have fixed the TSF to the input hypsometry, or we are not resampling the TSF - these parameters are defined in the hypsometry data file, as explained above).

You set the thermal history prior, run parameters and initiate a run in the same way as for non-detrital samples. The main difference in the output will be the graphical assessment of the output and in particular the predictions for the detrital data and the TSF (if this has been allowed to vary). This is shown below in the menu bar for **Summary Predictions**.

This shows the possibility to plot the detrital age and track length distributions (note the detrital length distribution option may not be accessible until you have plotted the detrital age distribution).

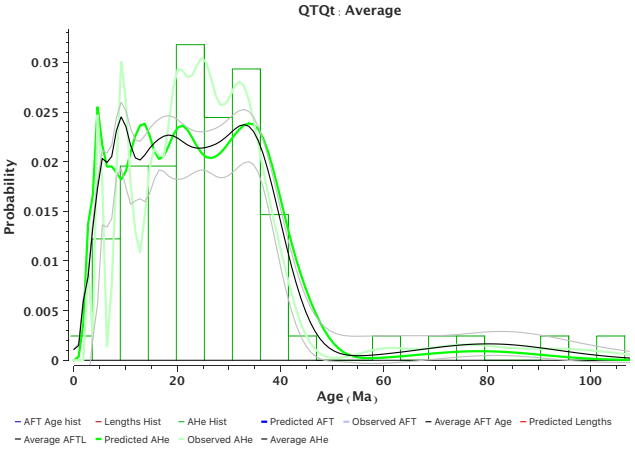
The 'Plot Detrital Length' button is not activated until you have clicked on the 'Plot Detrital Age' button. For

If you chose to plot the detrital age distributions, you will have a plot similar to that below (here with just AFT and AHe data).

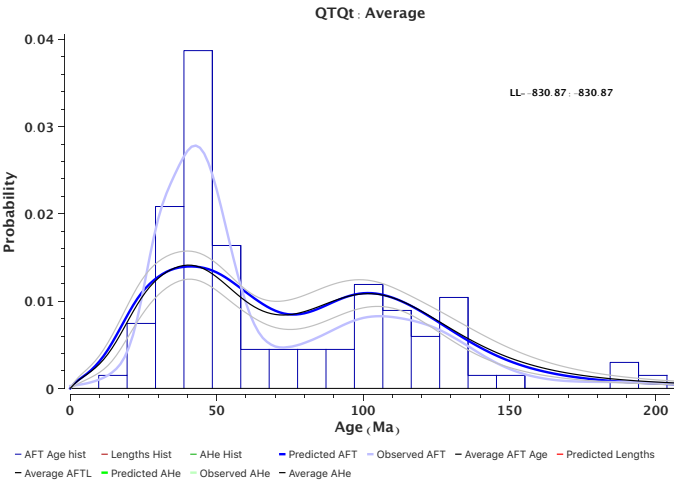


This shows the observed AHe (green) and AFT (blue) detrital age data in histogram and continuous distribution forms, as well as the predicted distributions (in the darker/heavier green and blue lines). The likelihood values shown on the plot will be the likelihood of just the detrital and the total likelihood (if we had also used in situ/bedrock data). In the example above, the two values are the same as we had not used in situ/bedrock data.

To plot AHe, ZHe, AFT alone, you can just click on the legend of the predicted curve you want to remove. For example, if we want to look just at the AHe data from the plot above, we want to remove the AFT data, so click on Predicted AFT in the legend, and you would then see something like



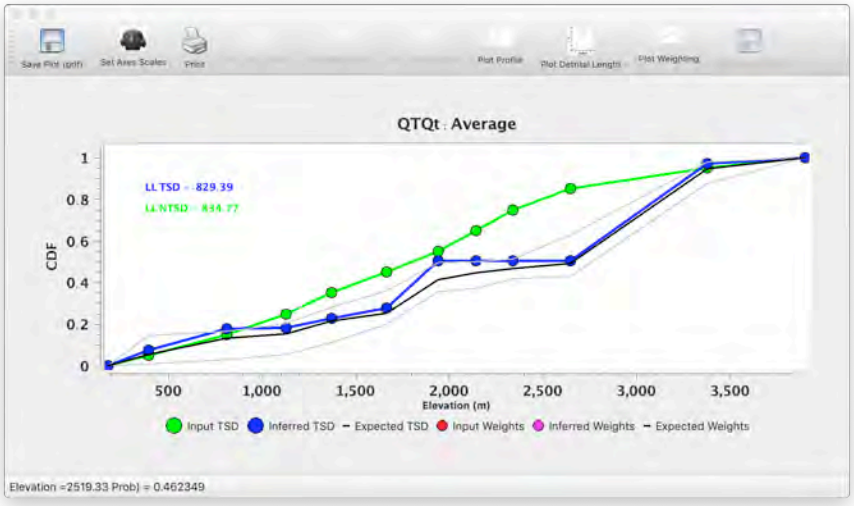
If we had clicked on Predicted AHe, we would have just the AFT data as below



Clicking on Predicted AHe restores the AHe data to the plot. We can similarly remove or add ZHe data.

In the case where we have allowed the TSF to vary, we can plot that too (plot TSD on the menu bar in the image below).

This will produce a plot similar to that below, where the green is the initial TSF (often the hypsometry) and the blue line is the inferred function, the black is the mean of all inferred TSF, with the 95% credible range shown by the thinner grey lines.



In the plot above, the TSF option on the menu bar has been replaced by **Plot weighting**. This is more or less the derivative of the TSF function, and represents the weighting applied to the predictions (e.g. age or track length distributions) at each elevation in the input hypsometry (the mid points in that elevations for which the weightings are constant in the plots below, except for the left and right hand side values in the plot, which are treated as the central points).


QTQt : Average
Weighting
0.5
0.4
0.3
0.2
0.1
0
500
1,000
1,500
2,000
2,500
3,000
3,500
Elevation (m)
Input TSD
Inferred TSD
Expected TSD
Input Weights
Inferred Weights
Expected Weights
Elevation =2427.6 Prob) = 0.229111

THERMAL HISTORY CONSTRAINTS MENU

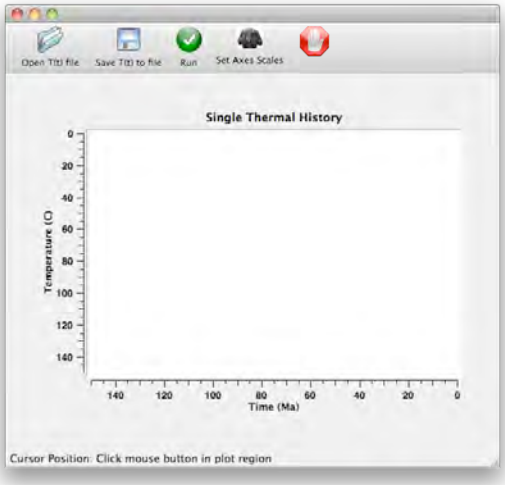
Required parameters are missing or incorrect.

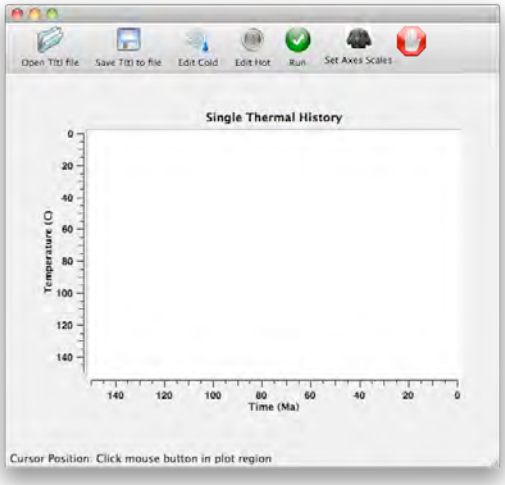
Before running the modelling, we need to set up the constraints on the thermal history relevant to all samples, and if required/desired any sample specific information. Thus, the run option is not available until we have at least chosen to set up a forward model or set the general thermal history constraints for an inverse modeling run. Also, to activate these menus, we need to have already opened one of more data files (as these contain data and information concerning the data we need for the modelling).

Draw forward thermal history

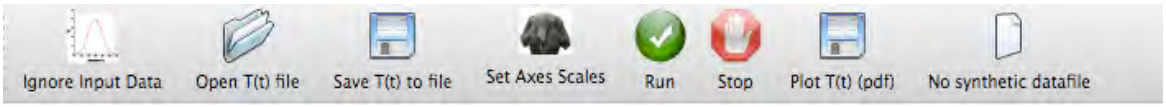
This allows us to use a graphics window to set up a forward model for one or more samples in a vertical profile. Note to run a forward model, we need to have read in one or more data files, as QTQt will use the same data types and certain input parameters (numbers of counts, lengths, grain sizes, radiation damage models, etc). You have the option to run a forward model, but to not plot these input data, so the actual input data themselves are then not important.

After selecting this option a window will appear, in the form of the one of the two possibilities shown below.





(Note as of version 5.6.3, the toolbar has been reordered and extended as below). Note the addition of the option to ignore the input data, which is explained on the next page.



If you have opened only one data file you will see the window on the left, while if you have opened more than one (for a vertical profile) you will see the window on the right.
In the second case, you will initially see the **Edit Cold** option in colour and **Edit Hot** greyed out. Here, Cold refers to the thermal history for the top (or shallowest) sample in a vertical profile, and Hot refers to the lowest (or deepest) sample. These two thermal histories (Cold and Hot) will have

the same number of time-temperature points, and the same time points. They only differ in the temperature values you assign.
The thermal histories for all samples between the top and bottom samples are determined by using the elevation/depth differences and linear interpolation of the temperature offset between the top and bottom thermal histories.

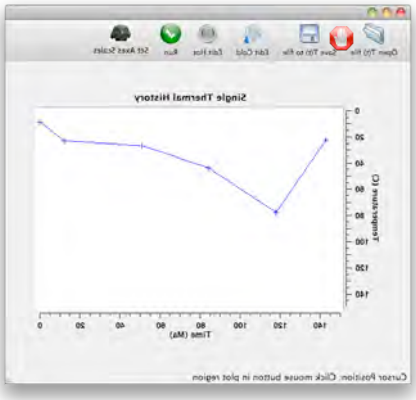
If multiple input data files contain stratigraphic information, then the stratigraphic age constraints will be plotted on the thermal history window. However, in the current version of QTQt (5.6.3) it is not possible to assign different time-temperature points to represent the stratigraphic age of each sample, as all thermal histories need to have the same number of points with the same times.

In version 5.6.3, the menu bar also has a button labelled **Ignore Input data** (which toggles to **Plot Input data**). This allows you to run a forward model, based on the data types and parameters from the input file(s), but to produce the output without plotting the input data themselves.

You have the option to save an input thermal history to a file (**Save T(t) to file**) , or open a previously created thermal history file (**Open T(t) file**).

Set Axes Scales allows you to change the range on the time and temperature axes.

We start the input the top thermal history by placing the cursor in the white part of the window. If you click the mouse and hold it pressed down, you will see cross-hairs in the window, and the time-temperature points given by the position of the cursor is written at the bottom left of the window. You select a point by releasing the mouse click. The thermal history will be drawn in blue, adding in each point as a '+' as you create them. The default minimum for the temperature axis is 0°C, but if you want to add a point < 0°C, you can just insert it with T > 0°C and move it as described below.

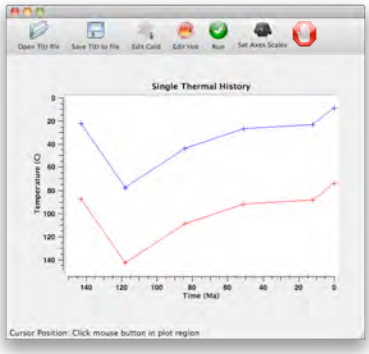


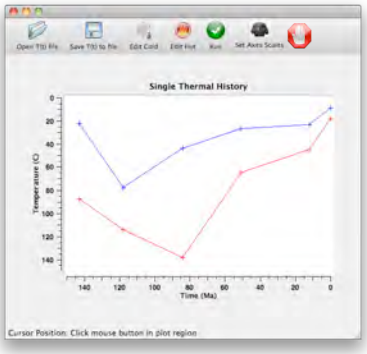
To **move** an already created point, place the mouse on the point, click and hold down the mouse and drag the point to the new desired location. You can move a point so its time value crosses (becomes older or younger) than an adjacent point.
To **delete** a point place the cursor on the point and double click.
Notes :
The time-temperature points can be input in any order (QTQt will sort them).
If you place the cursor at a time < 0.0, QTQt will set the time to 0.
If you do not input a point with time = 0, QTQt will add one, using the temperature of the closest time point.

When using a profile, you can then click on the **Edit Hot** button. Again you place the mouse in the window, and when you press and hold the mouse, you will see the time, temperature and temperature offset written at the bottom left of the window. The temperature offset is the difference in the temperature between the Hot and Cold thermal histories (i.e. the top and bottom samples in a profile).

Note : The temperature offset is not the same as the temperature gradient and the forward model runs described here will use ignore the option of using the temperature gradient. You can input temperature gradient value in a file (as negative values, see below) and these will be converted to the equivalent temperature offset.

You do not have to be too precise with the time coordinate as QTQt will just choose a point with the time closest to the mouse coordinate value. Choose any time point then click and and move the mouse (with the button held down) to get the offset you want. When you release the mouse, you will see a red thermal history drawn below the blue one, using a constant temperature offset (equal to the value selected for the point in the Hot thermal history (see figure below left). You can choose any point to set this constant offset value.
To edit points in the Hot thermal history to change from a constant temperature offset, again select and drag the point vertically and the point will change (see figure below right).





You can not change the time values not can you delete a point while editing the Hot thermal history). To do this you need to click on the **Edit Cold** option and move or delete the relevant time point for the cold (blue) thermal history.

You can input a thermal history from a text file using **Open T(t) file**. For a single sample the format is

N
t_1 T_1
t_2 T_2
.....
t_N T_N

where N is the number of time temperature points, t_1 T_1 is the oldest time-temperature pair and t_N T_N is the present day time-temperature pair (so $t_N = 0$). For a profile with multiple samples, the format is

N
t_1 T_1 O_1
t_2 T_2 O_2
.....
t_N T_N O_N

where O_1 is the offset temperature at time t_1 and O_N is the present day temperature offset, or temperature gradient (°C/km). If you want to use the temperature gradient in the file instead of offset,

enter the value as a negative number. The temperature gradient is then converted to an equivalent offset based on the maximum elevation difference in the data set.

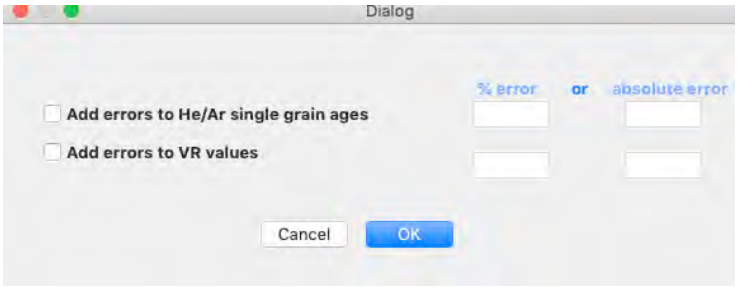
The input thermal history will be drawn to the screen and you can modify an input thermal history as described above.

The option **Save T(t) to file** lets you save the current thermal history to a text file.

Once you have created the forward thermal history for one or more samples, you can select the **Run** option and a new window will appear summarising the results (either for a single sample, or the predictions as a function of elevation/depth for a vertical profile).

If you have clicked on the **No Synthetic Datafile** button (the last on the toolbar, and this toggles to **Yes Synthetic Datafile**), QTQt will create a separate file with synthetic or simulated data for each input sample (data file), and the input thermal history.

If you have He or VR data and want to produce synthetic data with added noise, QTQt will prompt you for the input errors as below



The errors are dealt with in one of four ways.

(i) Input % error > 0 : this adds a systematic (positive) error equal to the % of the true predicted value

(ii) Input % error < 0 : this adds a systematic (negative) error equal to the % of the true predicted value

(iii) Input absolute error as value > 0 : this adds a Gaussian error sampled from a distribution with mean = 0 and with standard deviation equal to the input value

(iv) Input absolute error as value < 0 : this adds a Gaussian error sampled from a distribution with mean = 0 and with standard deviation equal to the input value (treated as a %) of true predicted value

For plotting the forward model predicted values for a single sample or individual samples in a profile, the plotting menu (Max. Likelihood Model) is active and can be used (see the later section on plotting).

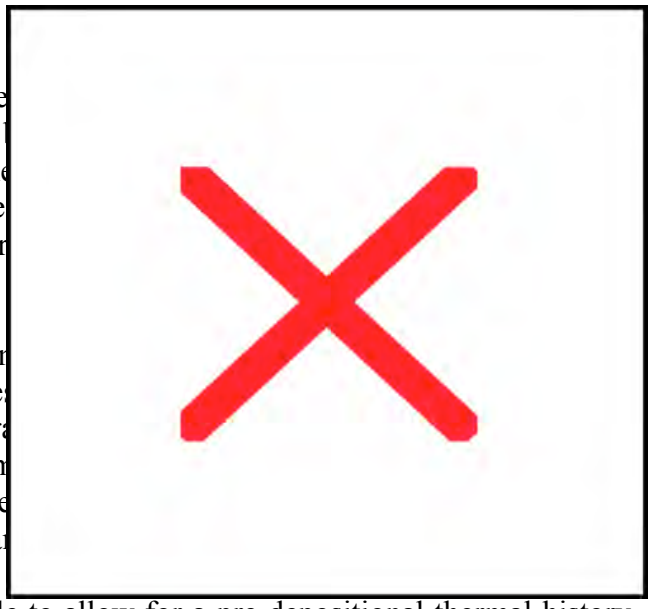
You can edit the thermal history and rerun a forward model as many times as you like. To stop this process, you need to click on the Stop button.

Note : when using sedimentary samples, the stratigraphic age is used as a constraint in the thermal history models (such that a given sample needs to be a surface temperatures at the time of deposition). This may then lead to the thermal history being different to that input using the graphical approach above. To confirm the actual thermal history used in the calculation, use the ***Plotting/Max. Likelihood Model/Thermal History*** menu option.

Inverse model prior

This allows us to set up information used in the MCMC sampling for the thermal history for one or multiple samples. A window similar to one of the two below on the left will appear. The window on the left is for the case with more than one sample (e.g vertical profile), and on the right for a single sample (the offset parameters are not used).

Required parameters are missing or incorrect.



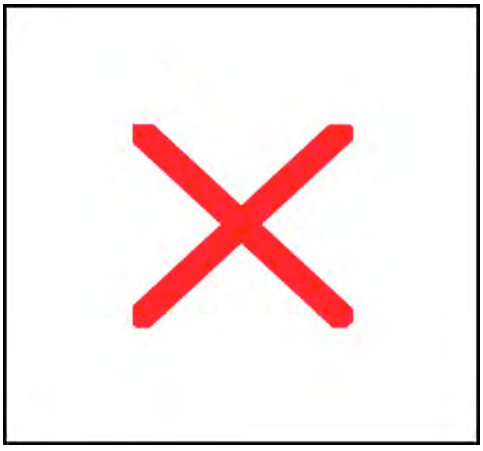
To set the **Ranges for General Prior**, we need to e
the time and temperature point in the middle of the
These are best set to be fairly broad. However, the
obtain as the broader the range, the more likely we
solution unless there is a lot of thermal history infor
MCMC works.

The window shows the oldest input age from all sar
constraints we might want to use. If the input file
age), then you will also see the oldest input stratigra
the range for the prior on time is set to have a maxim
the oldest input measured age, whichever is the olde
post-depositional thermal history for sedimentary sa

However, when dealing with sediment, it is possible to allow for a pre-depositional thermal history. This is modelled as 1 time temperature point older than the depositional age, and is independent for each sample. The default prior range on time for this pre-depositional time-temperaure point is equal to twice the range of the general prior.

Prior to version 5.6.0 QTQt limited the temperature to value >= 0.0°C (so no negative values are currently allowed). In earlier versions you will see that some of the entries in the thermal history dialog will change automatically to satisfy this condition. In version 5.6.0 and later, you can input prior ranges that allow temperatures < 0°C.

If you want to limit the rate of temperature change, you can set a maximum value, using the **Maximum $\partial T/\partial t$** option. This will limit both positive (heating) and negative (cooling) rates of temperature change.The default is 1000°C/my which is effectively no constraint.
In some case (e.g. when using sedimentary samples) it can be desirable to allow the constraint heating/cooling rate constraint to be exceeded over a limited temperature range. Once the default value is changed (to a value < 1000°C/my) you will see a slight modification to the dialog window, such that you can enter a maximum temperature difference (***Max <∂T allowed***) between two time-temperature points.



If a proposed model has a temperature change less than this value, then the rate constraint will be ignored.

To impose the desired constraint irrespective of the temperature change, set the value to 0 (this is the default).

When implementing this option, it can be useful to use smaller proposal scales for time and temperature than the default

values (see **MCMC RUN MENU**) to avoid rejecting too many models.

If you want to prevent reheating events, then click on the **No reheating** radio button. Note this no reheating constraint may be give inconsistent results (i.e. allow reheating) applied to samples for which you have entered a stratigraphic age (assumed to be sediments). Also, if you have entered present day temperature constraints in the data file for a given sample, the no reheating constraint may also lead to inconsistent results (or reheating) between to present day temperature from the preceding time-temperature point.

If you are using multiple samples in a profile, then the thermal history parameters you enter are relevant to the the highest elevation (or shallowest in a well) sample, i.e. the sample we expect to have experienced the coldest thermal history. For multiple samples, the thermal history for lower elevation (or great depth in a well) samples has the same form as that for the shallowest sample, but is offset by a value to be determined during the modelling. The offset parameters are the temperature difference between the lowest and highest elevation (or shallowest and deepest) samples over time. The thermal history for samples between these two is obtained by linear interpolation, based on the difference in elevation (or depth).

The elevation difference for the input data files will be written in blue below the present day temperature input boxes. You will see 2 values, the first value is the maximum elevation difference for all input files, and the second is the maximum elevation difference for the samples that will be used for the inverse modelling.

If you are running multiple samples, you will also need to set a prior range on the offset. If you have been running a single sample profile, then decide to use multiple samples, you might see the following dialog box.

Required parameters are missing or incorrect.

This is just to remind you that you need to see the **Temp offset** parameter prior range. If you do not, as an additional reminder, the OK button in the General Thermal History window will not be enabled. By default, the offset values for each time-temperature point are the same for all points, except the present day (but currently the same prior range in offset is used for the present day offset – the option to use a different range has not yet been enabled). If you want to let the offset vary between all time-temperature points, the you can check this option in the window**Required parameters are missing or incorrect.**. If you want to fix the present day temperature for various samples in a well for example, this is possible by using the **Individual Sample** menu, which we will come to below.

Once you have set the offset parameters, you will see the equivalent temperature gradient (°C/km) written in red below each parameter. If you have selected **Use temperature gradient for profiles** using **QTQt run and plot options** (**Plotting** menu), the offset set parameter will be replaced by temperature gradient (and you will see the equivalent temperature offset written in red below the input boxes).

If you have selected to ignore some input files for a profile with mutliple samples, then the default ranges for the temperature priors are based just on the maximum elevation difference for only the samples being used for inversion.

Finally, you can add in some constraints to the general thermal history that are applied directly to the highest elevation (or shallowest in a well) sample, and these are then imposed on the other samples by using the offset temperature. To do this either enter values defining a time-temperature box as described above and then tab to the next line to check the **Constrain** box (or you can check this box yourself before you enter the values.

Required parameters are missing or incorrect.

You can add up to 5 constraints (although this is a little against the spirit of transdimensional MCMC).

Note that you need to add these points is order of decreasing time (to the present day). However, these points are independent to the general thermal history prior described above (so can be older or younger or within the range defined by the general prior).

If you want to save the thermal history information to a file for later runs, you can do that by clicking in the button **Required parameters are missing or incorrect.**. You will be prompted for a file name.

If you want open a saved thermal history file, click on the **Required parameters are missing or incorrect.**. Again you will be prompted for a file.

The parameters are checked automatically to make sure they are valid (you can not enter negative values for examples) and the OK button will not be enabled untill all the relevant parameters have valid values.

Default values are loaded when the window first appears and if you want to use them you may have to just edit one value to enable the OK box.

Once you have entered at least the minimum information required for the thermal history (e.g. the general thermal history prior range and offset if required), the OK button will be enabled.

Individual Sample

If you are building a QTQt data file from scratch, or want to change some individual sample settings (such as the annealing model parameters), you need to use this menu option. A drop down menu will appear with the current loaded files (or the current run if you are building a new QTQt file). When you select a file, a window will appear as below.

This window summarises the information concerning the thermochronological data for the sample and lets you add sample specific thermal history information. The **Constrained point** option is intended to be used with sedimentary samples for which you know the stratigraphic age and temperature at the time of deposition (these can be input as a range). If this option is selected, then another time-temperature point is used in the modelling to allow for the pre-depositional thermal history. It is assumed that the temperature of this pre-depositional point is within the range specified for general prior of the total profile (see the next section for discussion of this) and the time is between the stratigraphic age and the maximum time specified for the general profile. Even if the post-depositional thermal history implies that the sample is totally annealed/degassed, this pre-depositional time-temperature point will still be incorporated (it is not a significant computational overhead).

The **Constrained Present day** option can be used to set the present day temperature to be within given limits (mean±range) for any sample. This is most likely to arise for well data. If the **±Range** parameter is set to zero, the value will be fixed at the **Mean** value.

Note that if you set the present day temperature or stratigraphic age for one sample in a borehole or vertical profile, you need to set these parameters for all samples.

You can set the **Annealing Model** for a particular run, and for the two Ketcham et al. models, you will need to set the **Compositional Model** parameter. **Value** is required according to the type of kinetic parameter you want to use. If you set the **Uncertainty** to 0, then the annealing model is chosen using this fixed value of the kinetic parameter. If you set the **Uncertainty** to a non zero value, then the compositional parameter is sampled from a normal distribution, with a mean equal to **Value** and a standard deviation equal to **Uncertainty**. This is one way to allow for uncertainty in the annealing models.
Allowing the annealing kinetic parameter to vary will also affect the annealing model used for radiation damage models applied to apatite He data. All the data in a given data file (e.g. AFT and AHe) will be modelled using the same value of the annealing kinetic parameter for a given iteration. If you want to allow the annealing kinetic parameter to vary for different AHe analyses from the same sample, you can do this by putting each analysis in a separate data file.
However, if you have only AHe data in a given file, and have chosen to vary either the He age, He error, or the eU value, the kinetic value will not be varied, but fixed to the input value.

You can set the Initial track length to a specified value. Note that for the Ketcham et al. (2007) annealing models, the default is to **Calculate initial track length** using the compositional information. You can uncheck this option if you do not want to do this. You can modify the annealing models parameters for **Use Projected lengths**, **Cf tracks**, or **Etchant** if desired, and the appropriate adjustment will be made to the annealing model predictions. Note if you use the Laslett et al. (1987) the options for Cf tracks, projected lengths, etchant, and the compositional parameters will not be used. The same applies to the 3 zircon models (and for these the appropriate default value for the initial track length will be inserted).

If the sample has He analyses, then the number of ages is summarised, together with the choice of alpha radiation damage model (one of : none, Gautheron, Flowers). Note this will be set to none if there are no U, Th and He concentration data enter for any analysis from a given sample as these are required for the alpha radiation damage modelling.

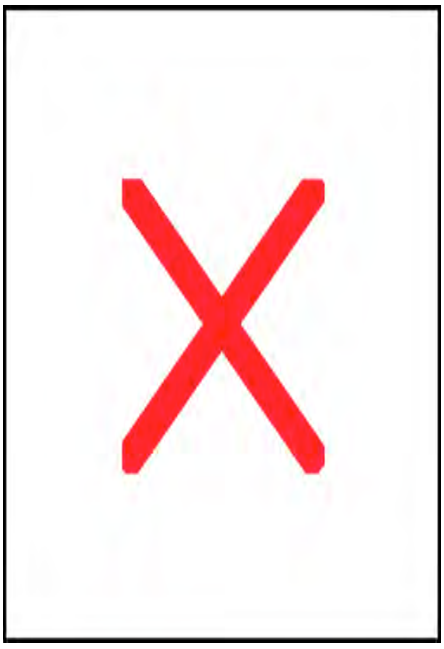
Finally, if you are building a QTQt file for the first time, or modifying an existing file, you can **Save data for reload**, and you will be prompted for a file name. If you do not select this, the changes will not be saved.
Note that the **Save data for reload** and **OK** buttons will not be enabled until valid input parameters have been set for the particular annealing model selected. This applies also for the thermal history constraints which must have positive temperature values.

MCMC RUN MENU

Required parameters are missing or incorrect.

This menu lets you set parameters controlling the MCMC sampling and run the sampler for thermal histories.

Set MCMC parameters
When you select this menu option, one of the two window below will appear depending on the version of QTQt:



On the left is for versions of QTQt prior to 5.7.0, and on the right version 5.7.0 and later.

The sampler for MCMC has 3 parameters to set controlling the number of iterations used in the sampling chain. The total number of iterations is equal to the **Burn-in** + **Post-burn-in**. The Burn-in is the number of iterations which will be discarded while the Post-burn-in is the number of iterations that will be used in subsequent inference of the thermal history. **Thinning** is a parameter that controls how many of the number of Post-burn-in iterations are used. If the parameter is set to 1, then all sample will be used, if it is set to 5, then every 5th sample will be used, if it is set to 10, then every 10th sample, etc. Larger values use samples which are further apart in the chain, and therefore less likely to be correlated. In general provided enough iterations are used, the thinning parameter is not too important.

There are no hard and fast rules about how to choose these except that they should be large enough that the inference is reliable (see Gallagher et al. 2009). While the values can be too small to have achieved satisfactory sampling, they can not really be too big, although larger values will increase the computation time accordingly. A qualitative check on whether the chain is sampled appropriately is to examine the likelihood or posterior values as a function of iteration. We will return to this later.

The other parameters to set are the proposal scales for moving **Time**, **Temperature** and (if relevant) **Offset**, for sampling the **FT annealing** kinetic parameters**, He Diffusion** controls reasmpling of He ages/errors and eU/Equivalent spherical radius and **Vitrinite Refl.** data/errors (if these options have has been previously selected when building a data file) and for **Birth** and **Death**, that is creating/deleting (referred to as birth/death) new time-temperature points (including offset if the offset is allowed to vary with time). For birth, the time is selected randomly between two existing time-temperature points and a temperature is calculated using linear interpolation between the two existing temperatures. The birth proposal scale **Temperature** is used to perturb this interpolated value. The same applies to the offset parameter if this is allowed to vary over time, using the **Offset** birth proposal scale. For moving the parameters, the scale parameters (in the same units as each parameter type) are in fact the standard deviation of a normal (Gaussian) distribution used to generate new values of the time, temperature or offset during the sampling chain. For the birth parameters, these represent either the standard deviation of a normal distribution or the width of a uniform distribution between –0.5 and 0.5. You can select one of those two options with the radio buttons, **Gaussian** or **Uniform**. The **Gaussian** option can propose models further from the current one than the **Uniform** option.

For version 5.7.0 the birth and death options (Gaussian or Uniform) are replaced by the options **if proposed outside prior** : **reject proposed** or **resample proposed**. The option **reject proposed** will always reject any model that is proposed with parameter values (e.g. a time-temperature point) outside the specified prior range. In this case, the proposed thermal history will always be rejected (in practice we do not even run the forward model). The option **resample proposed** will resample any parameter value proposed outside the prior until a valid value is proposed (that is, inside the prior). The other difference in version 5.7.0 is to **reject complex models that do not improve the data fit**. If selected (which is the default) this means when we add a time-temperature point to the current thermal history that does not change the way we fit the observed data, the (more complex) proposed thermal history will almost always be rejected. Similarly, if we remove a temperature point from the current thermal history and the data fit does not change, the (less complex) proposed thermal history will almost always be accepted. Accepting more complex models that do not change the likelihood tends to take longer to converge.

In terms of the default values for the **Time**, **Temperature** and **Offset** proposal scales, QTQt will estimate these based on the input thermal history model parameters. This is not to say that these will be the most appropriate values – these depend to some extent on the data themselves, and the information they contain about the range of acceptable thermal history models.

In the terminology of MCMC, we take the current model, choose a parameter from this model, then perturb that parameter (using a random sample from a normal or uniform distribution, centred on the parameter value of the current model, and a standard deviation equal to the value input here). This is explained further in Gallagher et al. (2009).

The remaining boxes in the windows are not enabled but will summarise the acceptance rates for the sampling (from the most recent sampling run). These rates will be between 0 and 1 and are useful to assess the performance of the sampler. The first 3 summarise the acceptance rates for the time, temperature and offset parameters. The birth and death terms reflect the acceptance rate for adding a new time-temperature point or deleting an existing time-temperature point respectively.

As with the number of iterations, there are no hard and fast rules about what values are optimal for the acceptance rates. However a general rule of thumb is a value between 0.1 and 0.7 is probably OK for the time, temperature and offset parameters. By changing the scaling parameters,

the acceptance rates for the thermal history parameters can be improved to lie within this range. In general, if you need to increase the acceptance rate, you should decrease the scale parameter. However, as the thermal history parameters are not independent (in terms of how they affect the better data fitting models), and also the prior ranges set on the time, temperature and offset parameters will influence the acceptance rate, then this not always true.

Note that if you are modelling a single sample, the offset parameter is not used and the acceptance rate is zero.

Run

This runs the MCMC sampler and you will see a standard progress bar to indicate where you are, as below.

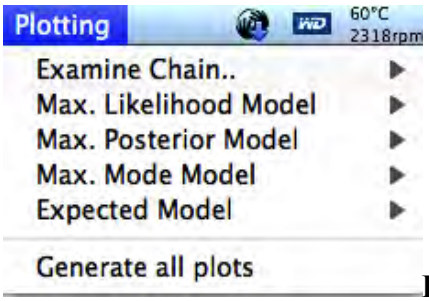
Required parameters are missing or incorrect.

You can cancel the run at anytime, and any subsequent inference or plotting will be made using the number of post-burn-in samples at the time you cancel the run.

Once the run is finished, you will see a window similar to the ***Set MCMC parameters*** window, but this time the acceptance values will be for the run just completed. This time however you can review the acceptance rates, and change the proposal scale parameters and/or the number of iterations if desired. This window has the option, **Save for Rerun**, to save these new parameters for a subsequent run. Normally, you will do this next run immediately. You need to click on the **OK** button and then use the **Run** menu option again. Note that if you change the parameters and do not click **Save for Rerun**, the changes will not be saved.

The boxes coloured pink and green indicate those parameters that have been modified as part of the MCMC sampling, while those greyed out have not been used (for example offset is not used for a single parameter).
The acceptance rates for the time; temperature and offset parameters should usually be around 0.2-0.5, with similar values for the FT Annealing, He Diffusion and Vitrinite Refl. sampling values, while the Birth and Death acceptance rates tend to be low (e.g. 0.005) , but in general should be more or less the same.

PLOTTING MENU



Required parameters are missing or incorrect.
Required parameters are missing or incorrect.
This menu allows you to examine various plots summarising the output from a given sampling run.

Each plot window has the menu options illustrated below

Required parameters are missing or incorrect.

By clicking on the appropriate image, a plot can be saved as an **editable pdf file** printed directly (and generally you can print to a pdf file, if you prefer this format), or you can change the axis scales from the original default values. You can also select SVG as the default plot format, using the plot and run options dialog window

Examine Chain
Required parameters are missing or incorrect.

These plots let you examine the performance of the chain in terms of the log likelihood (**Likelihood Chain**) or log posterior (**Posterior Chain**) as a function of post-burn-in sampling (blue curve, and use the left hand axis). On the same plot, you will see the number of time temperature points (green curve, and use the right hand axis). There should be no obvious trend in the likelihood/posterior (i.e. the mean value should be pretty much flat) and the values should change almost every iteration (i.e. it should not get stuck on the same value for too many iterations). Belwo the first panel shows a chain with poor convergence, while the other two are well mixed. Not the right hand panel is the posterior, and this tends to be lower as the number of model parameters increase.
Required parameters are missing or incorrect.Required parameters are missing or incorrect.Required parameters are missing or incorrect.

Max. Likelihood Model
Required parameters are missing or incorrect.
This option lets you examine details of the maximum likelihood model, that is the best data fitting model. The philosophy adopted here is that generally this model is likely to be too complex, that is it may have features which are not really justified from the data. However, it can be useful to examine the model.

Thermal History
This plots the maximum likelihood thermal history. There are no uncertainties associated with this single model.
Required parameters are missing or incorrect.

The figure shows an example of a thermal history for 3 samples in a profile. The blue curve is the reference thermal history (highest elevation sample), and the red curve is this plus the offset parameter (for the lowest elevation sample). Intermediate sample thermal histories are shown in grey, or for ignored data files their thermal histories will be plotted in yellow.
At the top of the thermal history plots, you will see a lost of buttons, as below.

Save plot (pdf) allows you to save the current plot to a file (either pdf or svg format, depending on the currently selected option for output files).

Set Axes scales allows you to modify the default values for the scales on the axes for the current plot.

Print allows you to print the current plot directly.

Save T-t to file allows you to output the thermal history in the current plot to a text file. For a single sample, this will be the number of time temperature points, followed by each time temperature pair in succession. For a vertical profile, you will see something similar to that below :

```
Reference sample  1
2 0 8 0
17.7679         37.553 110.266         110.266
0         0.434733         88.5848         88.5848
Standard sample  2
2
17.7679         43.4197
0         5.14789
Standard sample  3
```

The reference sample is the sample corresponding to the blue (cold) thermal history. If all samples are used for inverse modelling, this will be the top (highest elevation or shallowest depth) sample in the profile. If some samples ere ignored for inverse modelling, the reference sample is the highest elevation or shallowest depth sample used in the inversion. The other samples are identified as Standard samples. The next line has the number of time-temperature points, and some flags to indicate whether the modelling was made using temperature offset or temperature gradient, and the uppermost and lowermost samples used for the inverse modelling. This line is followed by the time, temperature and offset values for the current sample. If you want to use the thermal history for forward modelling, you just need to extract the number of time temperature points, and the time, temperature, offset values. For the standard samples, you will have just the number of time temperature points, followed by the time and temperature values (equivalent to the grey or red thermal histories in the plot above).

Sampled Like/Post
You can look at a selection of the individually sampled thermal histories. This will select 1000 thermal histories uniformly from the total number sampled post-burnin, allowing for the thinning factor. These will be plotted ranked in order of likelihood or posterior probability. These will be

plotted under the individual thermal history already selected and they can be removed by clicking on the same button. This can slow up plotting the actual thermal history you have selected (e.g. max. likelihood, max posterior, etc) as the plots are made at the same time (but only shown if you select the button). If you do not want this option, it can be turned off in the plot and run options dialog window.

Plot Individual predictions

This lets you select a single sample from the profile (using a drop down menu), and produce a summary plot of the observed data and the predictions from the maximum likelihood thermal history for that sample. This plot includes the track length distribution.

Required parameters are missing or incorrect.

Summary Model Predictions

This lets you plot the observed data (circles) and predicted values (cross for a single value, or continuous line) for FT age, FT MTL, He age, kinetic parameter and vitrinite reflectance as a function of elevation for all the samples in the profile.

Required parameters are missing or incorrect.

Note : For a sample with multiple He ages, there is a small perturbation added to the depth for each age (observed and predicted) to help discriminate between the different measurements.

You can also choose to plot the observed ages v the predicted ages – see the description of the Summary Model Predictions in the section on the Expected Model menu options.

Summary Information

At the moment, this option does nothing, but has been included for future developments.

Max. Posterior Model

This has the same options as described above for the maximum likelihood model, but for the maximum posterior model. The posterior probability is proportional to the likelihood multiplied by the prior. For models of constant dimension (i.e. the number of time-temperature points) and for uniform prior distributions (used in QTQt), the maximum likelihood and posterior models will be the same. However, QTQt implements a transdimensional MCMC sampler (the number of time temperature points is not fixed) Then the prior acts as a penalty against making the model too complex and the maximum posterior model will generally be simpler (less time-temperature points) that the maximum likelihood model. The choice of maximum posterior model is then sensitive to the range of the prior specified for the general thermal history model. The larger the range on the priors, the more we encourage the posterior models to be simple (i.e. the more we penalise models with a larger number of time temperature points).

Max. Mode Model
This model is obtained from the distribution of all models sampled. In 1-D, the mode is the peak of a 1-D probability distribution. If we divide the time-temperature space into squares with a resolution of 1 million year and 1°C, then for all temperature paths we can count how many temperature paths pass through each square. The mode model is the temperature value at each 1 million year step that has the most number of paths passing through it. The plot options for this model are described below (for the Expected Model).

Expected Model
In Bayesian formulations (as adopted in QTQt), the preferred single model is the Expected Model. This is effectively a weighted mean model, where the weighting is provided by the posterior probability for each model. This model contains features of all the models sampled in the post-burn-in sampling and in terms of complexity will generally lie between the maximum likelihood model (more complex) and the maximum posterior model (less complex). Also, we can use the MCMC sampling to calculate the uncertainty for the expected model and so draw meaningful credible intervals (more or less the Bayesian equivalent of confidence intervals). These intervals represent a 95% probability range for a given parameter, calculated so that 2.5% of the parameter values lie below and above the limits defined by the range.

The plot options for the Expected Model are a little different than the other two models. The drop down menu is below.
Required parameters are missing or incorrect.

Thermal History
The thermal history here represents the average of all the models sampled. If the profile contains more than one sample, then the uppermost sample thermal history will be plotted in blue, and the lowermost sample thermal history will be plotted in red. The thermal histories for all samples in between are drawn in grey. For the uppermost sample, the 95% credible intervals are draw in cyan (light blue) and these reflect the uncertainty in the inferred thermal history alone. For the lowermost sample, the 95% credible intervals are drawn in magenta and these reflect the combined uncertainty in the inferred thermal history and also the offset parameters. Any constraints will be drawn as black boxes.
Required parameters are missing or incorrect.

If you choose to save this thermal history to a text file, the output will include the upper and lower limits of the credible intervals.

Offset Temperature History
This is enabled only when there is more than one sample in the profile and plots the offset temperature (between the upper and lower samples in a profile) as a function of time. If the modelling was run with temperature gradient instead of temperature offset, the plot will show the gradient. During the MCMC run, the mean and standard deviation of the offset temperature is calculated as a function of time. The mean is plotted as a red line and the ± 1 standard deviation bounds as magenta lines. Also shown is the 95% credible range (a little like the ±2 standard deviation bounds) as green lines, calculated directly from the all post-burn-in samples in the MCMC chain.
Required parameters are missing or incorrect.

Plot Offset Histograms
This is enabled only when there is more than one sample in the profile and plots a histogram of the offset temperature parameter for either the present day or the palaeo-offset temperature parameter (only enabled if the offset parameter is set to be constant over time).
Required parameters are missing or incorrect.Required parameters are missing or incorrect.

Plot Individual T(t)
This plots the thermal history for a given sample (selected from the drop down menu). On this plot. The maximum likelihood and maximum posterior models are shown as a yellow and magenta lines, respectively. The expected model is shown as a black line, as are the 95% credible intervals. The latter are calculated directly from the probability distribution of the model parameter (i.e. the temperature at a given time) and can be asymmetric if the distribution is not symmetric. The black dashed lines are the credible intervals calculated as the expected model parameter ± 2 standard deviations (and so are symmetrical). Underlying these is a coloured plot showing the probability density of the thermal history (effectively the probability that the thermal history passes through a box of size 1°C x 1 million years or a time interval defined by dividing the current time range by 100). The probability scale is shown on the right of the plot, blue being low probability and red being higher probability. You can change the range on this probability scale by using the **Set Axes Scale** button.
Also shown on this plot are the maximum likelihood model (red), the maximum posterior model (magneta) and the mode model (white).
Required parameters are missing or incorrect.

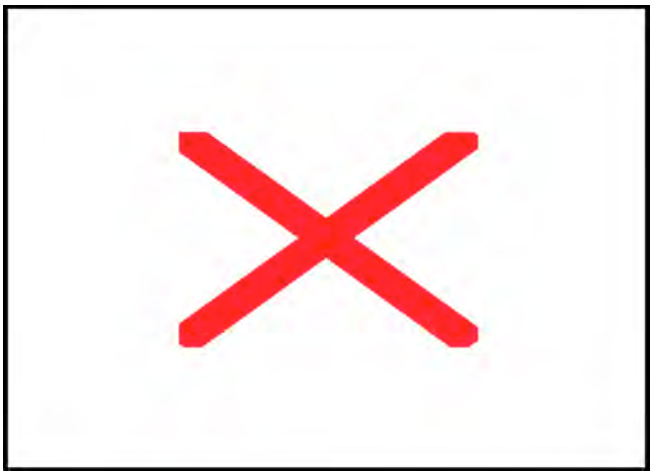
A new addition since v 5.2.2 is the option to produce a plot of the probability distribution of the temperature over a selected time range. On top of the individual T(t) , you will see a range of buttons,

and you can click on the button “Extract pdf of T(t)”. When you select this option the mouse will transform into a hand, and you can then choose a rectangle defined by the temperature and time range you are interested in. This will then produce a plot of the mean of the probability distribution for the temperature over the time range selected (in red) and the 95% confidence intervals about the mean.

You can select the button Return to T(t) to select a new time/temperature range.

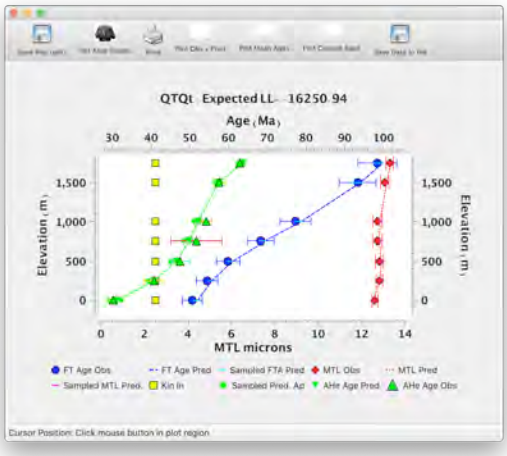
Plot Individual Predictions

This lets you select a single sample from the profile (using a drop down menu), and produce a summary plot of the observed data and the predictions from the expected thermal history for that sample. This plot includes the track length distribution (observed and predicted, with the 95% credible intervals on the predicted values). This plot also summarises the output of any sampling on the kinetic parameter and He ages (as described below). Each value is indicated by the following codes :
O = observed, P = Predicted, SP = sampled values of the Predicted value, SO = sampled values of the observed value.



Summary Model Predictions

This plots the predicted and observed values for all samples in the profile, as a function of elevation. Error bars with the same colour as the symbol are included on the observed values for each data type, when available. Also, the range on the predicted values is shown as a bar in a slightly different colour (for example, cyan for FT age, magenta for MTL, etc). This range summarises the mean and 95% credible range for the predictions from all thermal

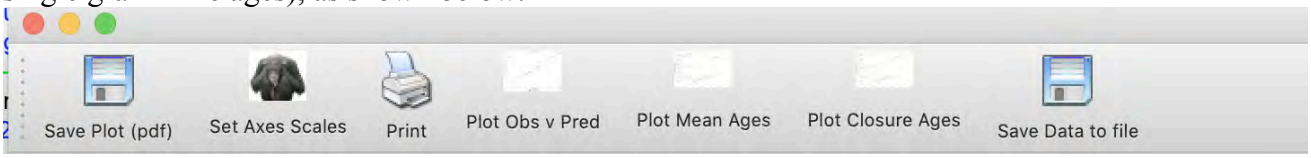


history models accepted during the post-burnin MCMC sampling.

You can remove a given type of data or prediction by double clicking on the symbol in the figure legend.

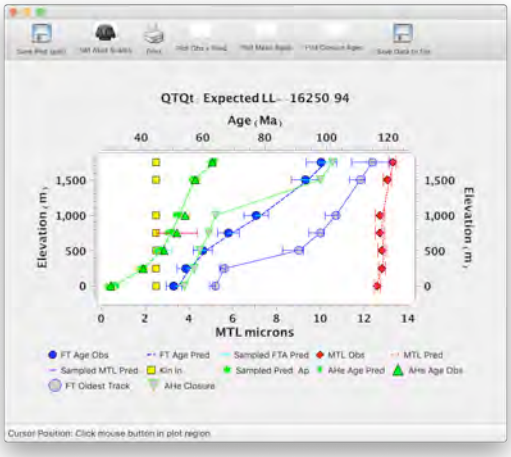
For some data types where are a given sample may have several measurements (e.g. AHe single crystal ages), a small perturbation is added to the elevation, to aid visual discrimination of different data points on the plot. This should result in the older ages for a given set of ages from one sample being plotted at a slightly higher elevations than younger ones.

In version 5.7.0 there is the option of plotting the mean ages for a given sample (e.g. for several single grain AHe ages), as shown below.



This mean is the calculated by weighting the individual ages by their respective error, as is the standard deviation of the mean. You can toggle back and forth between the mean and the single grain ages as the menu bar will be updated depending on what you have selected.

On this menu bar, there is also an option to **Plot Closure Age**. This leads to a plot similar to that below, in which the closure ages are shown as grey-filled symbols.

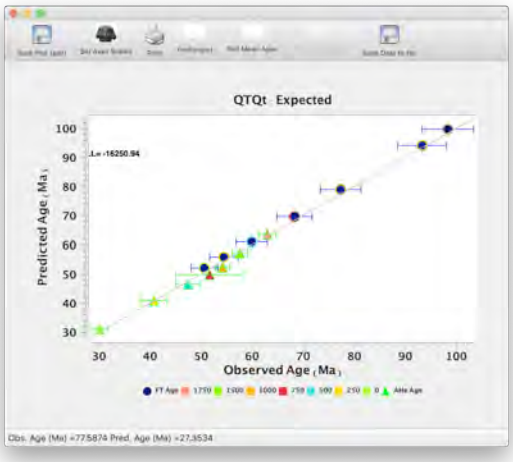


The **Closure Age** is calculated for a given thermal history for each AHe/ZHe grain and AFT/ZFT sample. For He data, it represents the time at which the grain was last totally degassed (and so would have had an age of zero). For FT data, it is the oldest time of formation of a fission track that has not been totally annealed and (in theory) could be observed today. This calculated **Closure Age** is then an indication (approximate) of the time at which a grain/sample cooled into the appropriate partial retention zone (PRZ) or partial annealing zone (PAZ) from higher temperatures. The **Closure Age** can then be used to assess how far back in time the thermal history is constrained/resolved for each grain/sample.

You can toggle the closure age off and on by clicking on the **Plot Closure Age** button in the menu bar.

If you have selected resampling of kinetics or age, then the plot output will show the ±2 standard deviation range of the accepted resampled values. This will be a horizontal line with x at each end in the same colour as the data type being resampled. The 2 standard deviation range of the predicted values will also be shown as a horizontal line with x at each end in a darker shade of the same colour.

There is also a button on the plot window that lets you select a plot of observed v predicted values, rather than as a function of elevation. This plot uses the same colour coding for different data types as the profile plot, but also adds a border around each symbol, choosing a different colour for each sample, and identifies the sample by its elevation/depth.
You can also plot the mean ages (predicted v observed) by clicking in the **Plot Mean Ages** button.
You can return to the profile plot by clicking on the Profile plot button.

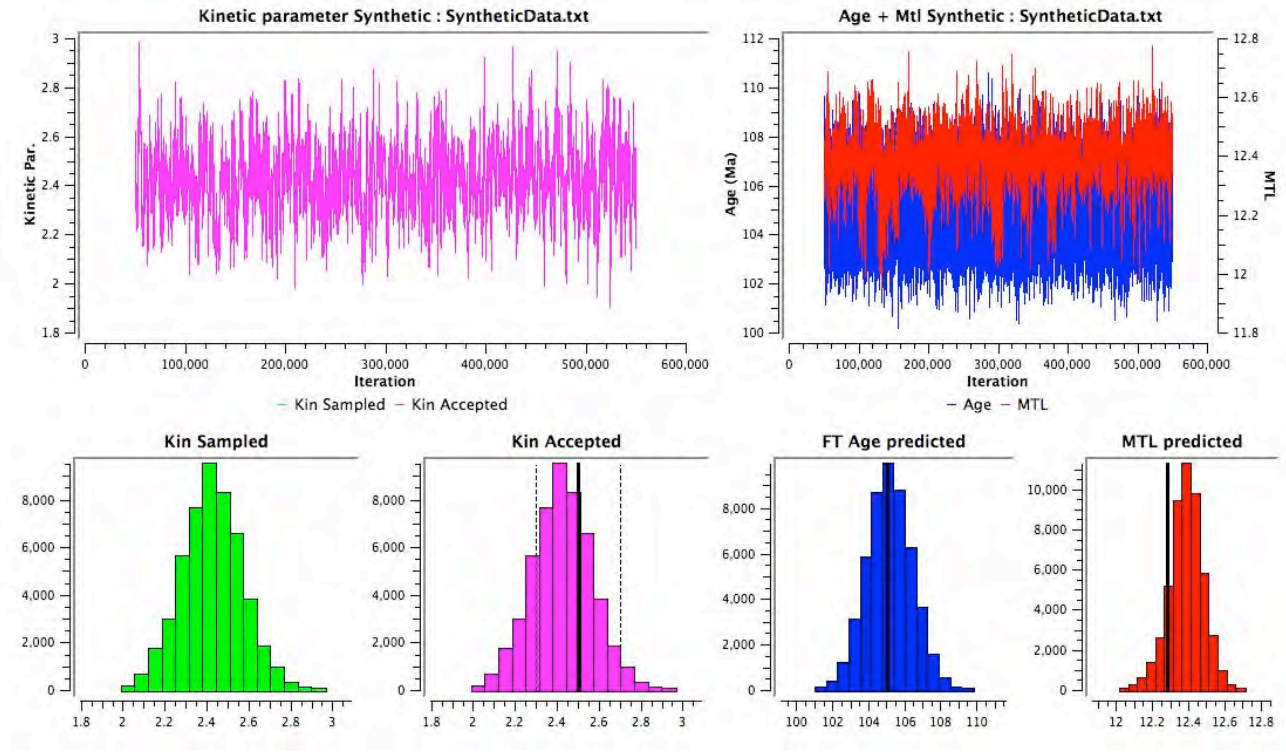


You have also the option to plot mean observed ages v mean predicted ages, or the vertical profile using the mean observed and predicted ages. This is useful for samples with multiple He ages or multicompositional AFT data for example and makes the plots a little less cluttered.

Note when plotting FT ages and MTL for multicompositional samples against the predicted values, the default is to plot the appropriate values for each compositional bin for each sample. When plotting the means, the values plotted are the weighted means, weighted by the number of counts (or track lengths) in each compositional bin. For the FT age, this weighted mean age is generally not the same as the central age, calculated from from the input Ns and Ni values. For the modelling, it is the Ns and Ni values that are used (in the likelihood calculation), while the weighted mean is just for graphical purposes/visual comparison.

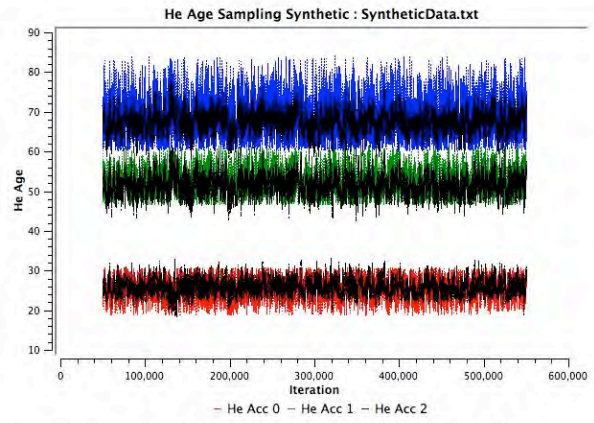
Plot Individual FT sampling

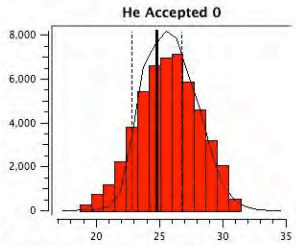
This allows you to examine the sampling of the FT compositional parameter, if this has been selected as a variable (by adding an uncertainty to the input value). Each sample can be examined individually. A typical plot is shown below. The top left panel shows the sampling of the kinetic parameter as a function of post-burn-in iteration (the proposed and accepted values, although often these are the same, as in the example below). The top right show the variation in the predicted FT age and MTL (note this also is a function of the thermal history). The lower panels show the distribution of the proposed (green) and accepted (magenta) values, the latter have the inut value with the ±1σ range, and the distributions of the predicted FT Age and MTL (with the black line indicating the input value).

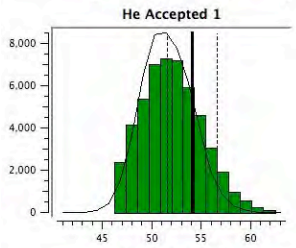


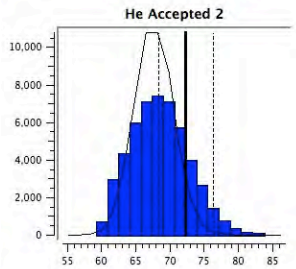
Plot Individual He/VR sampling

This allows you to examine the sampling of the He ages for a given sample. The top panel summarises the sampling as a function of iteration of each He age for a given sample (there will be on such plot for each group of 5 He ages). The coloured curves for each sample are the proposed and accepted He ages (the proposed are drawn as a dotted line) and black curve represents the predicted He age (a function of the thermal history). The distributions are summarised below for each He age in terms of the proposed distribution (left) and the accepted (right). On the latter you will see the input He age and its uncertainty (the black bars) and the distribution of the predicted He ages (the continuous black line) and the colour histogram represents the distribution of accepted values for each age.





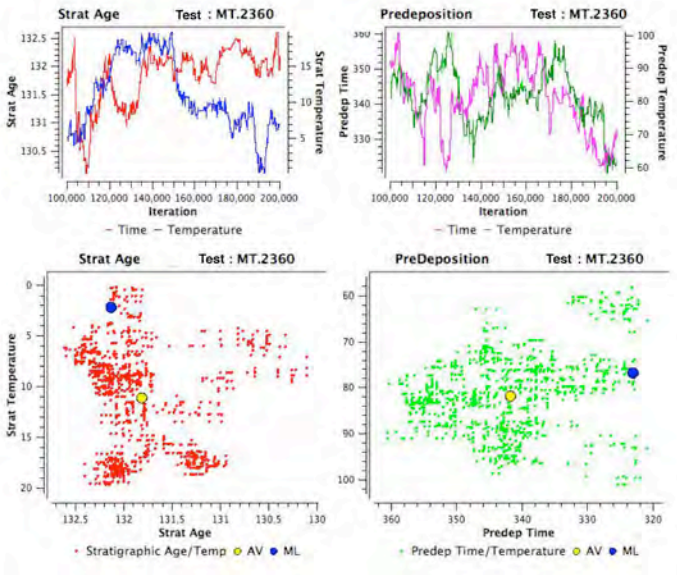




If hierachical sampling of the input data errors has been selected, then similar plot will be produced, but the variable plotted will be the estimated error scaling parameter for each datum that has been sampled.

Plot Individual PreDepositional sampling

This lets you examine the sampling of the stratigraphic ages/temperature and pre-depositional time/temperature points. The top two panels summarise these parameters as a function of post-burn-in iteration and the lower two, the joint sampling of time and temperaure (which is useful to assess any correlation). On these last two plots, the maximum likelihood (ML) and the expected (AV) model values are also given.



Summary Model Predictions

This lets you plot the observed data (circles) and predicted values for the expected model (cross for a single value, or continuous line) for FT age (blue), FT MTL (red), He age (green) as a function of elevation for all the samples in the profile. If the kinetic parameter has been varied, this will also be shown (yellow curve), relative to the axis for the MTL.

Summary Information
This option is not currently enabled.

Generate all plots
This option automatically generates and saves to files the available plots, except the plots for choosing a probability distribution on temperature over a selected time range from the thermal history. You may be prompted to save the run summary file (although this is not required , so you can select cancel). The files are saved to the directory where the QTQt application is running or to a previously selected directory. The file names will start with the run name you selected, and use the individual data file names where appropriate (the individual data predictions, and individual thermal histories for example). The final part of the file name indicates in a reasonably obvious fashion which plot it contains. The plot files will be saved as a single page as either editable vector pdf, SVG or JPEG format (for files with multiple plots in the same window). All files saved as JPEG are also saved as pdf with each plot on a separate page (the pdf files are of better quality).

Appendix 1. Example of QTQt input file format

OCO-04-07	**Sample ID**
0.1 0.2 198	**X, Y, Z co-ordinates (Z in metres)**
2 101 21 338.0 1.106e6 6131	**No of time temp points[1], $N_{lengths}$ N_{counts} zeta ρ_{dos} N_{dos}**
105	**code for annealing model[2]**
0 2.04 0.0	**code for composition, Value, error on value,[3]**
0 16.300000	**code for initial track length[4]**
0	**code for projected track data[5]**
0	**[6]code for Cf tracks**
1	**code for etchant [7]**
100. 10. 100. 10.	**Time, ∂time, Temp, ∂temp**
20. 20.	**Present Temp, ∂temp**
61.600 3.0	**FT age, error on FT age (Ma)**
12.80 0.1270	**MTL, error on MTL (microns)**
1.275 0.1275	**Std Dev, error on Std Dev(microns)**
61 135	**Ns Ni (must have N_{counts} values)**
.	
16.264987 30.0	**Individual track lengths (must have $N_{lengths}$ values),[8] and angle to C-axis (if available - see note 5) and compositional parameter (if available)**
15.561141 67.16	
.	
2	**No of AHe ages for the sample**
0	**Code for Radiation Damage Model[9]**
11.35 32.61 106.51 0.0 51.4 3 160.2 45.6 38.2	**He (ncc/gm or atoms), U, Th, Sm (ppm or atoms), Age (Ma)[10], error on age[10], Grain length, width, height (microns)[11]. The 2nd line below is α-ejection distance (microns), Do (m**2/s) and activation energy ($Jmol^{-1}$)**
20. 0.005 138000.0	
A 20. 0.005 138000.0 2 2 0	**A 2nd format in QTQt v5.4.1 and later allows the second line to include a mineral/isotope ID[12], and the last 3 are the Radiation Damage Model[9], mineral geometry[13], and % eU variation allowed (from 0 – 100%).**

[1] Apart from sediments, the time-temperature points can be set to 0. If you want to fix a stratigraphic temperature or time point within a specified ∂ range, set the ∂temp to a negative value. If you set the errors to zero. there will be a fixed time-temperature point. Remember these ∂ values are the half width of the range used to sample the time-temperature points.
Also, if the length data are in binned format enter a negative number for the number of track lengths. Enter 0 if there are no lengths

[2] **code for annealing models** :Apatite : 1= Laslett 1987, 100 = Ketcham multikinetic 1999, (102 = Laslett 1987 recoded by Ketcham), 105 = Ketcham multikinetic 2007, Zircon : 106 – Tagami et al. 1998, 107/108 – short/long time Yamada et al 2007)

[3] **code for composition**: 0 = Dpar, 1 = Cl (apfu), 2 = OH (apfu), 3 = Cl (wt%), 4 = r_{mr0} with $r_{mr0} + \kappa = 1.04$ (Ketcham et al. (2007).
Value is that appropriate to the composition code. If the error is non-zero, the value will be sample from a normal distribution centred on the value with a standard deviation equal to the error.

[4] **code** = 1 – calculate compositionally dependent initial length, 0 – use input value. You need to give a value of the initial length whether it is used or not

[5] **code** = ±1 for inputting c-axis projected lengths +1 means use the projected length model, -1 just to read the angles, but not use them, 0 for no angles, and 2 for already projected track lengths with no angle data

[6] **code** = 1 - Cf tracks, 0 – no Cf tracks

[7] **code** = 0 for 5.5 Molar (Donelick, A-Z), 1 for 5 Molar (almost everyone else).

[8] For binned length data enter 20 bin interval values (1-20) and the frequency for each interval

[9] **code** = 0 – no Radiation Damage, 1 – Apatite Gautheron et al (2009), 2 – Apatite Flowers et al (2009), -2 – Apatite Willett et al (2017) 3 –Zircon Guenthner et al. (2013), -3 Zircon et al. (2019). A value > 4 implies the model G2015, as implemented in Ricanati et al. (2017). Set to -1 for detrital data if you want to use the predicted age at the centre of the model crystal rather than the predicted whole grain age.

[10] **Age, error** – set age/error to a negative value to sampling from a distribution centred on the observed age/input error.

[11] The AHe data need to be in this format (i.e. the concentrations or number of atoms), but please use just the uncorrected age (and the error). Alpha ejection is dealt with when running the diffusion model.For the grain geometry you need 1, 2, or 3 values. I do the calculation for a spherical grain, which just requires the radius as the length parameter (set the width = height = 0.0). If you input the last height = 0.0, I assume this is equal to the width. I convert this to a sphere with the same surface are to volume ratio.
To sample the He age (or the error), set the input age (or error) to a negative value.

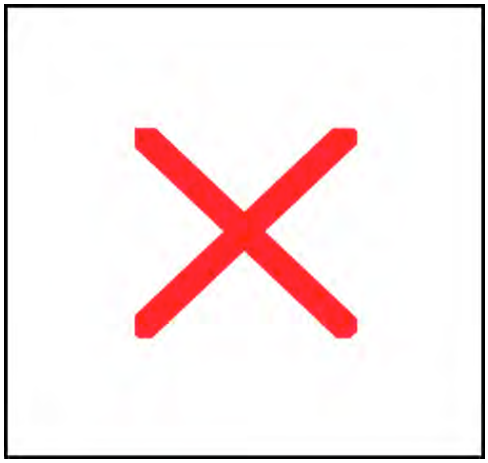
[12] A = apatite, Z = zircon, K = K-Ar/Ar age, O = other (for detrtital data, use the lowercase letter to not use data type in inversion)

[13] 2 = sphere , 1 = infinite cylinder, 0 = infinite slab

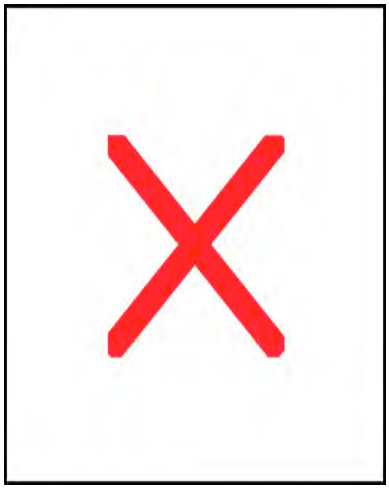
Appendix 2. Examples of typical input and graphical output from runs with the example files provided (note these results may differ from a run you make using these files).

(i) Single sample - QTQtExample.txt

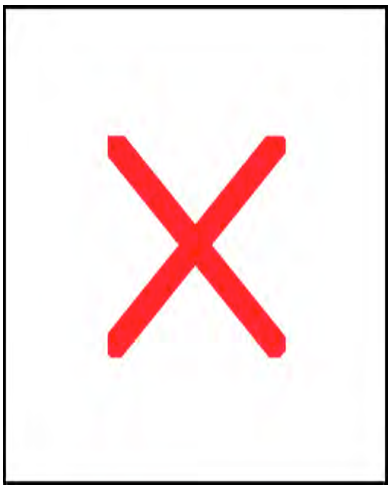
QTQtExample.txt



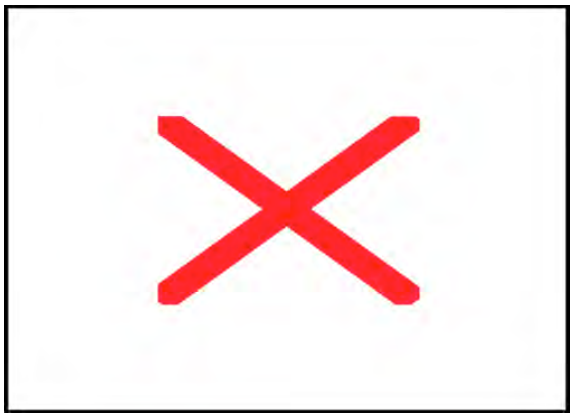
If you open this file, then select the **Thermal History Constraints** menu, you should see a window as shown to the right. Click OK and the select **Set MCMC parameters** (from the **MCMC Run** menu). You will see the window below with default proposal scales.

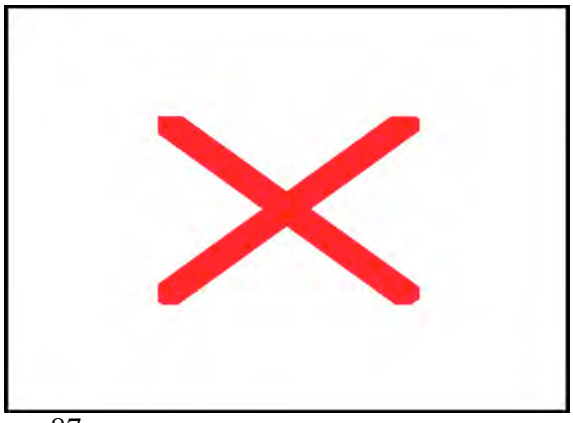


Click OK and choose **Run** (from the **MCMC Run** menu).
Once the run ios finished, you should see a window similar to the one below.



Here you can see the acceptance rates around 20-30% for the Time and Temperature, and typically lower values for the birth and death (but the two values birth and death are similar). You can change proposal scales and look at how the acceptance rate changes. If the scales are small then the acceptance rates tend to be higher, and vice-versa. This is not always the case as there is some interaction between the different parameters and MCMC moves.
However, if we continue, let us look at the sampling in terms of the likelihood (the fit to the data) as a function of the MCMC iterations. Choose the first option from the plot and you will see a plot similar to that below on the left.
The likelihood (blue curve) shows too much structure, which indicates that we need to do more iterations. In the plot on the right , we have the results of running 10000 iterations for the burn-in and 10000 post-burn-in.



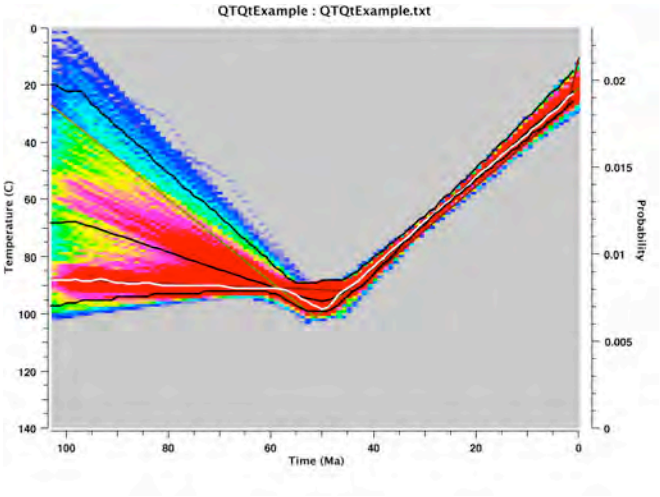


Finally if we run 50000 burn-in and 50000 post-

burn-in we have the results below. Here we see less structure as well as more sampling between different dimensions (or numbers of time-temperature points, the green curve). This is what we expect to see.

For this example, we can select the expected model thermal history (choosing **Plot Individual T(t)** from the **Plotting-Expected Model** and also the model predictions (**Summary Model Predictions** and **Plot Individual predictions**) we have plots similar to that below.

Required parameters are missing or incorrect.Required parameters are missing or incorrect.Required parameters are missing or incorrect.



(ii) Multiple samples

As a second example we will consider a vertical profile – the 8 files SynA1750HR.txt, SynA1500HR.txt ….to SynA0HR.txt represent samples at intervals of 250 m and each sample has AFT data and one AHe age. These data were generated with a thermal history equivalent to that used in Gallagher et al. (2005), their figure 3.

Using the default values for the Total profile thermal history constraints, the likelihood plot should resemble that on the left – again showing too much structure and not much transdimensional sampling. Running for 20000 iterations for the burn-in and 60000 post- burn-in gives us the plot on the right, and much better sampling. Overall, we can have too few iterations, but never too many (except for the amount of time it may take…). In this case the data are high quality and the solution is well constrained, so the burn-in period is relatively short.

Required parameters are missing or incorrect.
Required parameters are missing or incorrect.

Below are the plots for the **Expected Model – Thermal History** and **Summary Model Predictions**
Required parameters are missing or incorrect.
Required parameters are missing or incorrect.
Required parameters are missing or incorrect.
The thermal history starting around 110 Ma at temperatures below the total annealing temperature for the shallower samples implies rapid cooling from above these temperatures immediately before this time. If we add a constraint on the total profile thermal history, as shown in the dialog to the right (this constraint is possible as we know the solution). Running the profile data again, we have the results shown below. The fit to the data does not change much, and the form of the thermal histories after 100 Ma are similar. This shows there is little information in the data concerning the early part of the thermal history.

Required parameters are missing or incorrect.Required parameters are missing or incorrect.