Comparison of cooling histories constrained by two different fission track inversion models

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1. Introduction

The thermal history of a granitic rock body after its emplacement is generally controlled by the surrounding temperatures related to depth and geothermal gradient, especially in the low temperature range (e.g. «300°C). A significant rapid cooling episode revealed by a thermal history analysis is interpreted, in most cases, as an indication of rapid denudation soon after the regional uplift in the upper crust. Thermochronologic approaches including the fission track (FT) method have been widely applied in the study of the relationship between post-orogenic uplift history and its paleo-tectonic setting.

Although an apparent FT age contains mixed information derived both from older tracks with reduced lengths formed while temperatures were still in the partial annealing zone (PAZ) and from newer tracks with original lengths generated after the temperatures cooled below the PAZ, the FT method holds advantages for the thermal history analysis, because of its response to relatively low temperature ranges and its potential capability to make qualitative estimates of cooling patterns by examining the track length (TL) distribution (Gleadow et al., 1986).

TL reduction in apatite was quantified by controlled annealing experiments (Green et al., 1986) and presented as a mathematical equation as a function of time and temperature (Laslett et al., 1987). Based on the annealing equation and other additional experiments (Laslett et al., 1982; Green, 1988; Duddy et al., 1988), the forward modeling technique was developed to predict an apatite FT age and TL distribution for a

particular time-temperature (T-t) path (Green, 1989). In practice, additional thermal history information is needed to model observed FT data.

Corrigan (1991) suggested a possible solution to the inversion problem using the Monte Carlo method, and since then several inversion programs for thermal history analysis have been developed and subsequently modified (e.g. Gallagher, 1996; Willett, 1997; Ketcham et al., in press). Various inversion modeling software are widely available for FT data interpretations in many geological settings (e.g. see section III in Van den haute and De Corte, 1998), however, the algorithms for random T-t path generation and the ideas to represent the solutions are slightly different from each other. Although each of them has been built based on different concepts and has both strength and weakness, the comparison between different inversion modeling systems at the same standing point as a user (who attaches the importance to the parameters pre-set and/or recommended by the program developers) would help to avoid the overestimation of analytical results. We happen to have a chance to use two software packages developed by Willett (1992) and Ketcham et al. (in press). Here a series of thermal history analytical results derived from different inversion modeling programs presented.

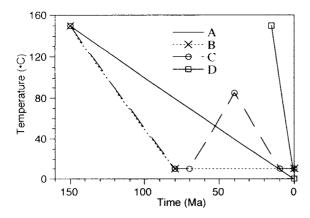
Methodology

The Controlled Random Search (CRS) algorithm originally developed by Willett (1992), later slightly modified by Issler (1996) and the AFT Solve (AFTS) developed by Ketcham et al. (in

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_	Modeled apparent apatite FT age (Ma)							
Synthetic T-t path	CRS	AFTS						
Α	98.9	97.8						
В	130.2	129.5						
C	112.8	111.2						
D	11.4	11.3						

Fig. 1. Forward modeling comparison between CRS and AFTS. Each model FT age corresponds to the various synthetic T-t path shown on the left.

press) are similar to other inversion modeling systems, in that they are mainly composed of the random (or semi-random) T-t path generators using the Monte Carlo method, combined with forward modeling and statistical tests to evaluate the goodness of fit by comparing the observed and modeled FT data.

Although algorithm details and computation techniques are described in the original studies (Willett, 1997; Ketcham et al. in press), we here briefly summarize several aspects of each inversion models and describe the pre-set values used in this study.

2. 1 Forward modeling

It is necessary in forward modeling to integrate the annealing processes over time with the continuous creation of new tracks. The forward modeling technique is developed based on the following process in a manner similar to that described by Green et al. (1989); (1) divide the thermal history into a series of small discrete isothermal segments (or substeps) to approximate the original thermal history to the desired level of accuracy; (2) calculate the amount of annealing for population generated during each substeps using the annealing equation (e.g. Laslett et al., 1987; Willett, 1997) and the concept of equivalent time (Duddy et al., 1988); (3) approximate each of the track populations as a Gaussian distribution; (4) sum up all track populations with various weights to account for the relative contribution to the distribution; (5) calculate the age contribution of each track population assuming the relationship between FT density reduction and TL reduction (Green, 1988) and sum these to predict a model FT age.

In this study, the time was divided into 100 isothermal segments for both the CRS and AFTS based on the detailed discussion by Issler (1996).

At the heart of the forward model is the annealing equation which calculates reduction ratio for a set of time and temperature. Laslett et al. (1987) presented the Arrhenius model based on the most complete data set collected through a series of controlled annealing experiments for induced FTs in the apatite (Green et al., 1986). Although Durango further annealing equations with modifications have been suggested since then (e.g. Crowly et al., 1991), Green et al. (1989) indicated that the fanning Arrhenius model of Laslett et al. (1987) best predicts the observed FT age and TL data derived from the Otway basin, Australia, especially for samples which have undergone only a small amount of annealing and which have similar chemical compositions to the Durango apatite. The fanning Arrhenius model of Laslett et al. (1987) is used by the AFTS, while the CRS uses a slightly different equation (Willett, 1992) derived from an additional modification of Crowley et al. (1991).

In both the CRS and AFTS models the track populations generated during each substep are summed with two weighting factors. The first is to correct for a sampling bias factor that is caused by the decreased possibility that shortened FTs will be revealed by etching, and are excluded from the length measurement (Laslett et al., 1982). The other accounts for the decrease in track generation due to the depletion of ²³⁸U through geologic time. The AFTS sums all track populations from present day towards past, which is in the opposite sense of the most of other forward models including the CRS, and the computational speed is

greatly improved.

Because the forward model directly controls the inversion results, consistency in forward modeling between the CRS and the AFTS must be examined. Perhaps the best way to do this is compare the modeled FT ages for various synthetic T-t paths, because FT ages are the final product of forward modeling and are implicitly influenced by all the processes involved, such as TL reduction and the summing of weighted track populations. Fig. 1 indicates the comparison of modeled FT ages for various T-t paths from Willett (1997), and the corresponding FT ages predicted by AFTS for the same T-t paths. Although FT ages predicted by the AFTS tend to be slightly younger than those from the CRS, the difference in modeled FT ages derived from all T-t paths, representing a wide variety of cooling rates and cooling patterns, is negligibly small (about 1%) compared with the associated statistical error of an observed FT age.

2. 2 Inversion modeling

Since consistency between the two forward models has been confirmed, we now briefly describe the inversion approach. Inversion modeling is a process of seeking a set of thermal histories supported by the observed FT age and TL distribution that is carried out using the following procedures; (1) generate a great number of random T-t paths using a Monte Carlo method; (2) predict the model FT age and TL distribution for each generated T-t path with forward modeling; (3) compare the modeled FT data with the observed data and keep the only T-t paths which fit at the selected statistic level.

Each random T-t path generated by both the CRS and the AFTS are presented as several line segments joining T-t nodes which are mobile only in temperature direction, hence temperature is the only variable parameter after selecting the number and the time intervals for the nodes. In this study, twelve nodes with intervals of 10 million years through time were selected for the CRS, while the eight nodes with uneven time intervals were chosen for the AFTS.

The genetic algorithm used by the CRS (similar to Gallagher, 1996) is the Monte Carlo search method with a strategy for increasing the search efficiency until convergence occurs by localizing the search space into a reasonable region after purely

random generation of anumber of T-t paths. First, an initial random set of 250 (50-300 were suggested by Willett, 1997) T-t paths are generated. Next, a new T-t path is generated with searching the regions close to the mean of initial set. If the new model FT age and TL distribution correspond to the new T-t path fit the observed data better than any of those previous paths, new T-t path is added to the set and the worst fitting T-t path in the set is thrown away. This process is repeated until all 250 T-t paths pass the statistical test at the desired confidence level (normally 95%).

This strategy is not adopted for the AFTS random T-t path generation, because its improved computational efficiency makes it possible to generate a much larger number of purely random T-t paths and maintain a similar running time to the CRS. After selecting the total number of T-t paths to generate, all T-t paths pass the statistical test are retained. For both the CRS and AFTS, an envelope of acceptable solutions is generated which indicates minimum maximum temperature estimates at each fixed time. Fig. 2 indicates 250 acceptable T-t paths derived from the CRS inversion analysis, and displays the way in which acceptable envelopes (e.g Fig. 4, 6 on the left) are formed in both CRS

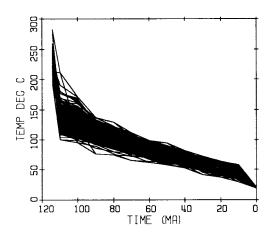


Fig. 2. 250 T-t paths accepted at 95% confidence level derived from CRS inversion modeling for sample (10). Acceptable envelope is formed by connecting each of time-node which represents on the upper or lower temperature limit.

and AFTS analyses. Note that each upper and lower boundary obtained by connecting all nodes at each time are not required to pass the statistical test. For comparison, we selected a total of 7,500 T-t paths for the AFTS analysis to obtain the acceptable envelope formed by 250 T-t paths, since it was previously found that about 1,500 acceptable T-t paths were generated after 40,000 iterations.

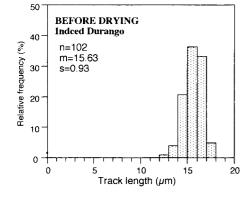
The FT age and TL distribution is used to evaluate the goodness of fit for each T-t path. The Kolmogorov-Smirnov (K-S) test (Press et al., 1988; Gallagher, 1996) is used to judge the agreement between observed and modeled TL distributions in both the CRS and AFTS analyses. The modeled FT ages are evaluated against the absolute value of misfit weighted by the standard deviation of error in the observed FT age in the CRS (Willett, 1997). The K-S test is also used to compare the modeled observed FT ages in AFTS (Ketcham et al., in press).

To represent the solutions resulting from inversion analyses, the AFTS chooses the one T-t path which shows the best fit to the observed data based on the K-S test, whereas the CRS calculates the exponential mean thermal history of the all T-t paths in the solution set (although the CRS also produces the best fit T-t path, this is not used for further interpretation in most cases). The use of mean solution tries to emphasize the point that all accepted T-t paths support the Additionally, the meaningless fluctuations of individual T-t paths can be eliminated by using the exponential mean thermal history. Although this approach has some advantages, exponential mean is limited in that it assumes that the solution set is unimodal. The modeled FT ages and TL distributions corresponding to the exponential mean solution do not agree with the observed FT data relative to the best fit solution by AFTS.

2.3 Data for the inversion models

The data set used for the comparison of the two inversion models were obtained for the Mesozoic granites in the Dahingganling Mts, northeast China. Although Himeno et al. (1997) preliminary reported the zircon and apatite FT ages and apatite horizontal confined TL distributions for the same samples, the apatite FT ages and TL distributions were re-determined for the newly mounted grains with the following experimental modifications. All apatite grains were mounted in Petropoxy resin hardened after heating at 120°C for 40 min. Thermal neutron irradiation for apatite FT dating was carried out at a reactor which shows higher cadmium ratio (Au Cd≫ 3). Etching for apatite TL measurements was done by using 5M HNO3 at 24°C for 25-30 seconds as recommended by Dr. Ketcham (in communication). Apatite confined TLs measured at the total magnification of x2000 using Zeiss Axioplan microscope equipped with a projection tube and a digitizing pad.

Before apatite TL measurements for northeast China granite samples were done, the induced TL for the Durango apatite standard (previously totally annealed at 500°C for 8 hours) was measured to normalize the experimental procedures. However, anomalous slightly shortened tracks were observed (Fig. 3, left) which was caused by residual fluid in the etched tracks. Therefore, all the apatite length mounts were wiped with ethanol and heated for 4 hours at 140°C to remove the fluid, revealed the further distinct track ends (Fig.3, right). This raised the possibility that relatively high number of shortened TLs reported in Himeno et al. (1997) were partly a result of residual fluid in the etched tracks. The mean induced TL (=16.17 μ m) derived from Durango apatite after removing the residual fluids was used as the initial TL value in the AFTS inversion analysis.



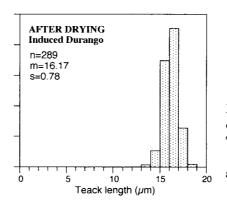


Fig. 3. Induced FT length distributions for Durango Apatite. The initial mean length of 16.17 μ m was used in the AFTS analysis.

Table 1. Zircon and apatite FT ages and apatite confined Tls used in this study.

Sample	Zr FT age	Ap FT age	Ap TL data		Mean length in 1 μm bin													
	±1 σ (Ma) (#of grains)	±1 σ (Ma) (#of grains)	No. of Tracks			5.0≤	6.0≤	7.0≤	(- ·			racks 11.0≤				15.0≤	16.0≤	17.0≤
(10)	114±13	78.0±9.0	112	12.73	2.40	5.41	6.66	7.43	8.74	9.51	10.51	11.57	12.48	13.53	14.46	15.33	16.53	-
	(7)	(30)				(2)	(4)	(3)	(3)	(3)	(6)	(3)	(21)	(32)	(23)	(11)	(1)	(0)
(14)	117±16	102±6	145	13.68	1.36	-	-	7.20	8.17	9.84	10.73	11.40	12.57	13.53	14.45	15.37	16.09	-
	(5)	(30)				(0)	(0)	(1)	(1)	(1)	(2)	(7)	(23)	(43)	(48)	(18)	(1)	(0)
Synthetic	-	101	104	13.8	1.2	-	-	-	-	_	10.5	11.38	12.31	13.27	14.23	15.19	16.13	17.00
(14)						(0)	(0)	(0)	(0)	(0)	(1)	(4)	(16)	(30)	(30)	(18)	(4)	(1)

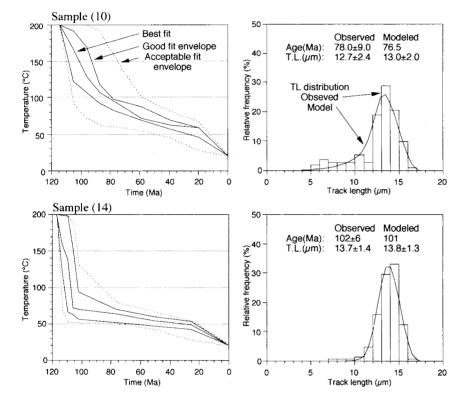


Fig. **AFTS** inversion modeling results. 'Best fit' Tt paths well as good and acceptable fit envelopes are shown on the left. Modeled FT ages and TL distributions correspond to the best fit T-t path are on the right to compare with observed data. Although modeled FT data for T-t paths included in good envelope show theoretically distinguishable limit of K-S test (=0.5), the modeled FT data for 'best fit' T-t path numerically shows the lowest value of objective function and the least disagreement with the observed data judged by K-S test after 7500 random T-t paths generation.

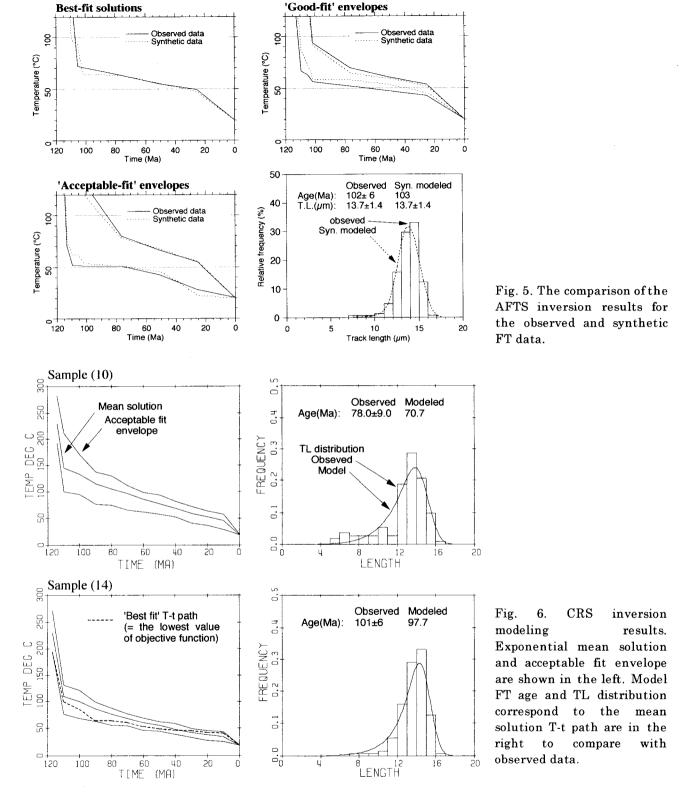
Zircon and apatite FT ages and apatite confined TLs used in this study are shown in Table 1. The synthetic (14) data in Table 1 were produced by approximation of the modeled FT data (bottom right in Fig. 4) corresponding to the best fit T-t path derived from the AFTS analysis (bottom left in Fig. 4) and used for the additional modeling below.

3. Analytical results and discussion

Fig. 4 (left) shows AFTS inversion modeling results of 'acceptable fit envelope' at 95% confidence level (including about 300 T-t paths) and the 'best fit' T-t path after generation of 7500 random T-t paths. The additional boundary, 'good fit envelope' shown in Fig. 4 (left) is composed of all T-t paths which fit the observed data better than

the statistical limit of the K-S test. The comparison between the observed and modeled FT age and TL distribution corresponding to the best fit T-t paths, are shown on the right in Fig. 4. Apatite inversion models only constrain thermal history between 120and 50°C corresponding to the apatite PAZ (e.g. Wagner and Van den Haute, 1992).

To obtain an idea of the analytical limitations, the best fit T-t path for the sample (14) was assumed as a 'known' thermal history and additional AFTS inversion modeling was carried out using the synthetic data (Table 1) in order to examine the validity of best fit solution from the AFTS analysis. The comparison of AFTS inversion analysis for both the observed and the synthetic data is shown in Fig. 5. Although this additional



inversion analysis has not been carried out using the CRS, at least the synthetic data for the best fit solution from the AFTS analysis reproduce the initially observed FT data fairly well (bottom right in Fig. 5). However, a maximum difference of 20°C at 105Ma was seen between two best fit solutions. This demonstrates that an almost infinite number of T-t paths can exist at the time of rapid cooling

from temperatures high enough to cause total annealing between about 110 and 100Ma. Thus the inversion results probably are not best represented as a single solution, and further interpretation should be be made in consideration of the 'acceptable' or 'good fit' envelopes as representative of the limit of our ability to model the thermal history using inversion analysis.

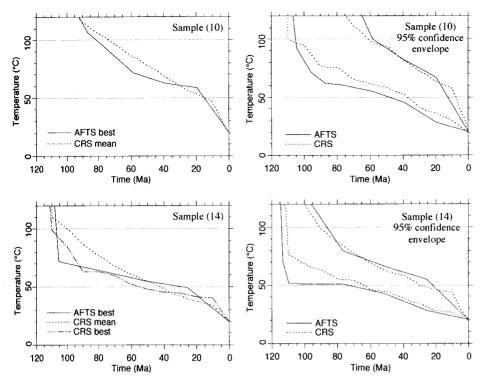


Fig. 7. Detailed comparison between CRS and AFTS inversion results. The 'best 'mean' T-t paths and solutions are shown on th left. the acceptable envelopes at 95% confidence level are on the right. Both of best fit T-t paths and mean solutions agree well for sample (10). Although both inversion results for sample (14)indicate the rapid cooling temperature pattern. 105 Ma difference at around 40°C.

Fig. 6 (left) shows the CRS inversion modeling results for the exponential mean solution and the acceptable fit envelopes composed of 250 T-t paths (Fig. 2) which fit the data at 95% confidence level. The comparison between the observed and modeled FT ages and TL distributions corresponding to the exponential mean solution is shown on the right in Fig. 6. Note that the scale of the Y-axes in Fig. 6 (left) is different from that in Fig. 4(left).

Before we make a comparison between the CRS and the AFTS results, it should be mentioned that the CRS dose produce a bounding envelope which is equivalent to the AFTS good fit envelope by choosing the 0.5 significance option. However, we didn't select the 0.5 significance option for the CRS analysis because almost all studies using the CRS so far had been carried out in the same condition as in this study (e.g. Willett et al., 1997; Glasmacher et al., 1998) and also it consumes much longer running time relative to the AFTS.

There is a general good agreement between the CRS and AFTS algorithms, and characteristics of the cooling histories predicted by both analyses are similar, e.g. rapid cooling between 117 to 110Ma followed by slower cooling for sample (14), whereas a more linear and slow cooling below 120°C for sample (10). Furthermore, modeled FT ages and TL distributions corresponding to the CRS exponential mean solutions and the AFTS best fit T-t paths seem to reproduce the observed

data fairly well. A detailed comparison of the results, however, reveals the differences in some parts of the modeled cooling histories.

A comparison in terms of reproducibility of the observed data (Fig.4, 6 right) suggests that the CRS approach results in a relatively larger disagreement between the observed and modeled FT ages and TL distributions, as clearly seen in the modeled FT ages. The primary reason for this is that a 95% confidence level was chosen to accept T-t paths in the CRS analysis, but the AFTS results includes 'good fit' T-t paths which matched the observed data above the distinguishable limits permitted by the K-S test, in other words above the level not supported by the limits of the data quality. An additional reason is that the mean solution is a somewhat manipulated T-t path which is not one of the 250 solutions in the solution set, even if it is supported by 250 acceptable T-t paths.

Fig. 7 shows a direct comparison of the solutions predicted by the CRS and the AFTS. Note again that the maximum vales of Y-axis are 120°C corresponding to the highest temperature constrained by apatite inversion analyses. The 'best fit' T-t paths derived from the AFTS and the 'mean' solutions from CRS are shown in the left and the 'acceptable fit' envelopes are shown on the right. Both the 'best fit' and 'mean' solutions as well as the acceptable fit envelopes agree fairly well for sample (10) with maximum temperature

differences of only 10°C. In contrast, the best and the mean solutions and acceptable fit envelopes disagree for sample (14) from 110 to 80 Ma. A disagreement is particular seen the temperature at 105 Ma for sample (14). The best fit T-t path from the AFTS analysis suggests a temperature of 70°C at 105Ma following the rapid cooling, whereas the mean solution from the CRS shows 110°C. The comparisons of both inversion models for the sample (10) and (14) suggest that the use of mean solution is the reason to introduces a significant disagreement with the best solution at a period when the constrained thermal history shows a rapid cooling like the result for sample (14). In other words, if the mean solution instead of the best fit was used in AFTS. the predicted thermal history between 110Ma and 100Ma would be completely different and the temperature at 105Ma might result in around 115°C because the upper and lower accepted limits are 51°C and 185°C, respectively.

In summary, fairly good agreement was found in the thermal histories predicted using the CRS and the AFTS algorithms, the differences suggest the necessity to indicate whether the obtained thermal history is the 'best fit' solution or the 'mean' solution, although each has advantages. The most important factor in terms of the reliability and limitation of inversion modeling is the consistency of bounding envelope at a selected confidence level. The 95% acceptable fit envelopes from the AFTS was found to be slightly larger than those of the CRS at 95% acceptable fit envelopes in a limited series of modeling. Although this may suggest that the genetic algorithm used in the CRS generates relatively less random T-t path because of its two step strategy, the pre-settled values, such as number and intervals of time nodes for inversion modeling, also affect the results of modeling and the further work is required.

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