GEOLOGICAL SURVEY OF CANADA
COMMISSION GEOLOGIQUE DU CANADA

Open File 2325

AN INVERSE MODEL FOR EXTRACTING THERMAL HISTORIES FROM APATITE FISSION TRACK DATA: INSTRUCTIONS AND SOFTWARE FOR THE WINDOWS 95 ENVIRONMENT

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EXECUTIVE SUMMARY

Apatite fission track thermochronology has become a powerful and popular method for reconstructing low temperature (<150°C) thermal histories for a wide range of geological environments. This report provides executable programs and instructions for using a constrained random search inversion modelling technique for extracting time-temperature history information from apatite fission track data. The modelling procedure described herein was developed at the Geological Survey of Canada and is based on a modified version of the inverse model, TINV52, created by Sean Willett. The Introduction provides some background on how the model evolved. This is followed by a section on installing the program which specifies hardware requirements and provides a listing of all necessary files and computer programs. A third section outlines the function of each program and describes important modifications to the model. The final section gives detailed instructions for executing the sequence of programs that comprise the model. Appendix I contains a list of key model parameters, definitions and recommended parameter choices. Example file structures, model outputs and plots are included in appendices II-IV. Appendix V contains a description of the time step predictor function used to integrate the fission track annealing equation and the appropriate coefficients for each annealing model included in AFTINV32. The FORTRAN programs have been compiled to run under the Windows 95 operating system and 32-bit Windows NT windowed executable versions are included as part of this report.

ACKNOWLEDGEMENTS

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INTRODUCTION

The roots of this computer model go back to the period from 1989 to the early 1990's when Sean Willett was doing post-doctoral studies in the Department of Oceanography at Dalhousie University. The Dalhousie University Fission Track Research Laboratory was quite active by then and was involved in some major fission track studies. It was recognized that, with recent advances in the understanding of how fission tracks anneal in apatite, it was appropriate to develop an objective method of quantitatively analyzing fission track parameters for thermal history determinations. Sean developed a constrained random search inversion model for calculating a range of thermal histories that provide statistically acceptable fits of calculated fission track age and length parameters to the observed data. This model has been used in a number of studies involving the Western Canada Sedimentary Basin (Issler *et al.*, 1990; Willett and Issler, 1992; Ravenhurst *et al.*, 1994) and a modified form of it, as described in this document, is being used currently at the Geological Survey of Canada for a wide range of studies. The original model has been described briefly in the above publications and readers should refer to them for details of the modelling philosophy. A more detailed description of the model can be found in a recent paper prepared by Willett (personal communication). Essentially, the inverse model uses the forward model of Willett (1992) to perform track annealing calculations.

Sean's original model (TINV52) was not designed to be used by others and, as a result, it was difficult to set up a model run. This document describes how I have modified the model to make it into a more user-friendly package. An interactive program, TSORT32, was written to sort raw track length files in order of increasing length for use by the inverse model. An interactive front end program (PREAFT32) was created for setting up model parameters. However, because the model is flexible and allows for a variety of user inputs, users must choose their parameters carefully. Logic checking is imbedded in the code to ensure logical consistency between user-specified temperature and rate bound limits. If poorly chosen parameters are used, the inverse model is forced to stop if calculated temperatures fall outside of the pre-determined limits. The modified inverse model, AFTINV32, includes changes in both how random thermal histories are calculated and how the annealing calculations are performed. Many of the changes, including the way the program was compiled, have resulted in decreased model run times. An interactive post-processing program (POSTFT32) was written to summarize model results and create plotted output. The next sections describe briefly how to install the program, what the various model components are and how to go about running the model.

Disclaimer: Although every effort has been made to test this modelling software, it cannot be guaranteed to be "bug-free" and users must accept any problems that arise from its use (or misuse). This series of programs will be subject to occasional future modifications designed to improve on model processes and to incorporate any additional advances in fission track studies that are relevant to modelling (e.g. changes in annealing kinetics as a function of composition). The current version uses the empirical annealing equation of Crowley *et al.* (1991) (see Appendix V) but users do have the option of changing the annealing model coefficients.

INSTALLATION

i) Hardware Requirements: The computer code has been optimized for use with the Intel Pentium processor on a PC that is using the Windows 95 operating system. The program will perform well with a 486 processor but, in terms of reasonable model performance, the recommended minimum requirement is a 486 PC running the Windows 95 operating system.

ii) Directory Structure: Create the following directory structure, giving the source directory some appropriate name. All pertinent files are contained on the 3.5" micro floppy disk which accompanies this report.

a) Source Directory: Copy the following 8 files into the source directory.

(FORTRAN executable programs and a batch file for plot generation)

TSORT32.EXE
PREAFT32.EXE
AFTINV32.EXE
POSTFT32.EXE

ZPLOT.EXE
ZPPOST.EXE
ZPVIEW.EXE
GOFTPLT.BAT

b) Subdirectories: Copy the listed files into the input and data subdirectories. These are default files which can be overwritten and renamed, if desired. AFTMOD.BIN contains parameters for a specific model run and is generated on execution of PREAFT32. All the files in the output and plot directories are created during execution of the sequence of model programs. The modelling procedure is illustrated using an example with real apatite fission track data. Appendices II-IV contain data and input files (Appendix II), output files (Appendix III) and plots (Appendix IV) for the example provided.

INPUT
(Model parameters)
AFTPARM.IN
AFTSPL.IN
AFTPLOT.PAR
AFTMOD.BIN

DATA
(Track/age data)
TRACK.IN
TRACK.SRT

OUTPUT
(Model outputs)
PREAFT.OUT
INFO
POSTAFT.OUT
TINV.S05
TINV.SOL
TRACK.OUT

PLOT
(Plot files)
PDF05.PL
AVETMP05.PL
MINTMP05.PL
ALLTMP05.PL
CLOSAG05.PL
ALLPDF05.PL
AVET.DXF, .PS
ALLT.DXF, .PS
MINT.DXF, .PS
PDF.DXF, .PS
CLOS.DXF, .PS
ALLPDF.DXF,.PS

Programs

All programs containing the number 32 have been compiled as 32-bit Windows NT windowed executable programs using Watcom FORTRAN 77 version 10.6. These programs are designed to run on a PC which uses the Windows 95 operating system. See Appendix I for definitions and recommended choices for key model parameters. Appendix II-IV contains relevant files and output for an example model simulation of real apatite fission track data. Appendix V describes the time step predictor function used to solve the empirical apatite fission track annealing equation of Crowley *et al.* (1991) with coefficients for the following apatite compositions: Durango apatite (Crowley *et al.*, 1991; Laslett *et al.*, 1987) and Sr fluorapatite and fluorapatite (Crowley *et al.*, 1991).

TSORT32 Program sorts track length data in order of increasing length using the Quicksort algorithm (Press *et al.*, 1986). It slightly modifies any equal lengths to make them unequal and appends the fission track age ± one sigma (supplied by the user) to the sorted track length file (see Appendix II for example files). Track length data **must** be sorted before it can be used by the inverse model program, AFTINV32. Default input: DATA\TRACK.IN (unsorted file); default output - DATA\TRACK.SRT (sorted file), OUTPUT\TRACK.OUT. The file, TRACK.OUT, contains a record of any initially equal track lengths which have been modified by TSORT32.

PREAFT32 This is an interactive FORTRAN program which sets up parameters for an inverse model run. AFTPARM.IN contains general parameters for the annealing model (e.g. model coefficients, initial track lengths, etc.) and for controlling and monitoring the progress of the random search inversion method. AFTSPL.IN contains specific parameters which are relevant to the particular fission track sample being modelled (e.g. rate, temperature bounds, model times). Both AFTPARM.IN and AFTSPL.IN contain brief descriptions of model parameters (see Appendix II for example files) and can be edited directly although it is easier to use the interactive editing features of PREAFT32 to view model parameters and set up a model run (**Note: don't alter the format if directly editing either file or PREAFT32 will not be able to read them**). Both files can be renamed and overwritten during execution of PREAFT32. Parameters for the current model are written by PREAFT32 to the binary file AFTMOD.BIN for use by the inverse model AFTINV32. Output from PREAFT32 is written to PREAFT.OUT which is located in the output subdirectory. PREAFT.OUT contains title information and a record of selected model parameters for a specific model run (see Appendix III for an example file).

AFTINV32 This is a modified version of Sean Willett's inverse model, TINV52. The program generates a set of random forward model thermal solutions which are used to calculate apatite fission track age and length parameters for comparison with observed data. Predicted cumulative track length distributions are assessed with respect to observed lengths using the Kolmogorov-Smirnov statistic and a pass/fail criterion is established at the 0.05 significance level. Predicted fission track ages are required to be within two standard deviations of the measured age. The initial set of random thermal solutions is updated iteratively, with better-fitting solutions progressively replacing the poorest-fitting members of the set, using a constrained random search inversion technique (Figure 1). The model converges when all members of the retained solution set pass the statistical test.

The original program, TINV52, has been extensively modified to become AFTINV32. Some of these changes include reducing the size of the main program, adding new subroutines, converting from double to single precision, modifying file structures and drastically reducing the number of output files. This new version includes an integration time step size predictor function (Issler, 1996) to speed up program execution by adjusting isothermal step sizes according to heating/cooling rate and maximum interval temperature (Figure 2; also see Appendix V). Model time intervals are discretized into an integer number of substeps by dividing each time interval by the parameter, DELSUB, the time for track component generation (tracks in each component are assumed to be of constant age and behave as single populations of induced tracks in annealing experiments). Program execution time is sensitive to the value of DELSUB because this parameter controls the number of substeps and limits the size of isothermal step used by the program. For example, when DELSUB is small (e.g. 2 m.y.), it can be the

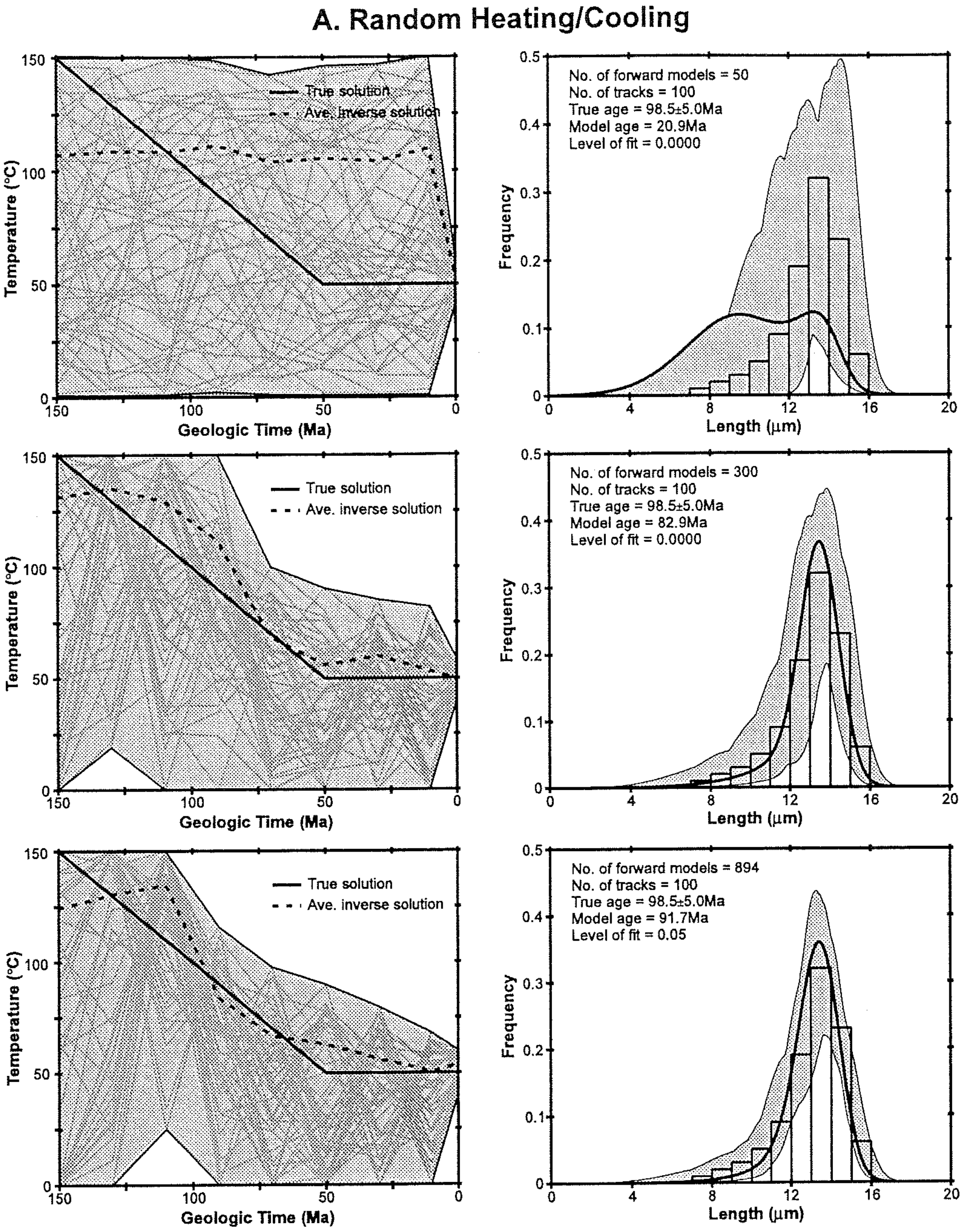


Figure 1. Illustration of constrained random search inversion method using synthetic apatite fission track data generated from the true temperature solution (heavy black line on temperature-time plots) for a) random heating and cooling and b) random cooling only thermal histories. In the upper left panels, an initial random set of 50 solutions is created (light grey lines in shaded regions). During continued iteration, successive members of the initial set are replaced by improved solutions (middle left panels) until all members of the set are statistically valid (convergence at significance level probability of 5%) (lower left panels). The preferred thermal solution (dashes) is represented as an exponential mean of all solutions contained within the acceptable solution space (grey shading). The corresponding calculated track length distribution for the mean temperature solution (heavy black curve in right panels) is shown in comparison with the synthetically generated distribution (histogram). The shaded regions on the length distribution plots indicate the range of track distributions produced by the random temperature set.

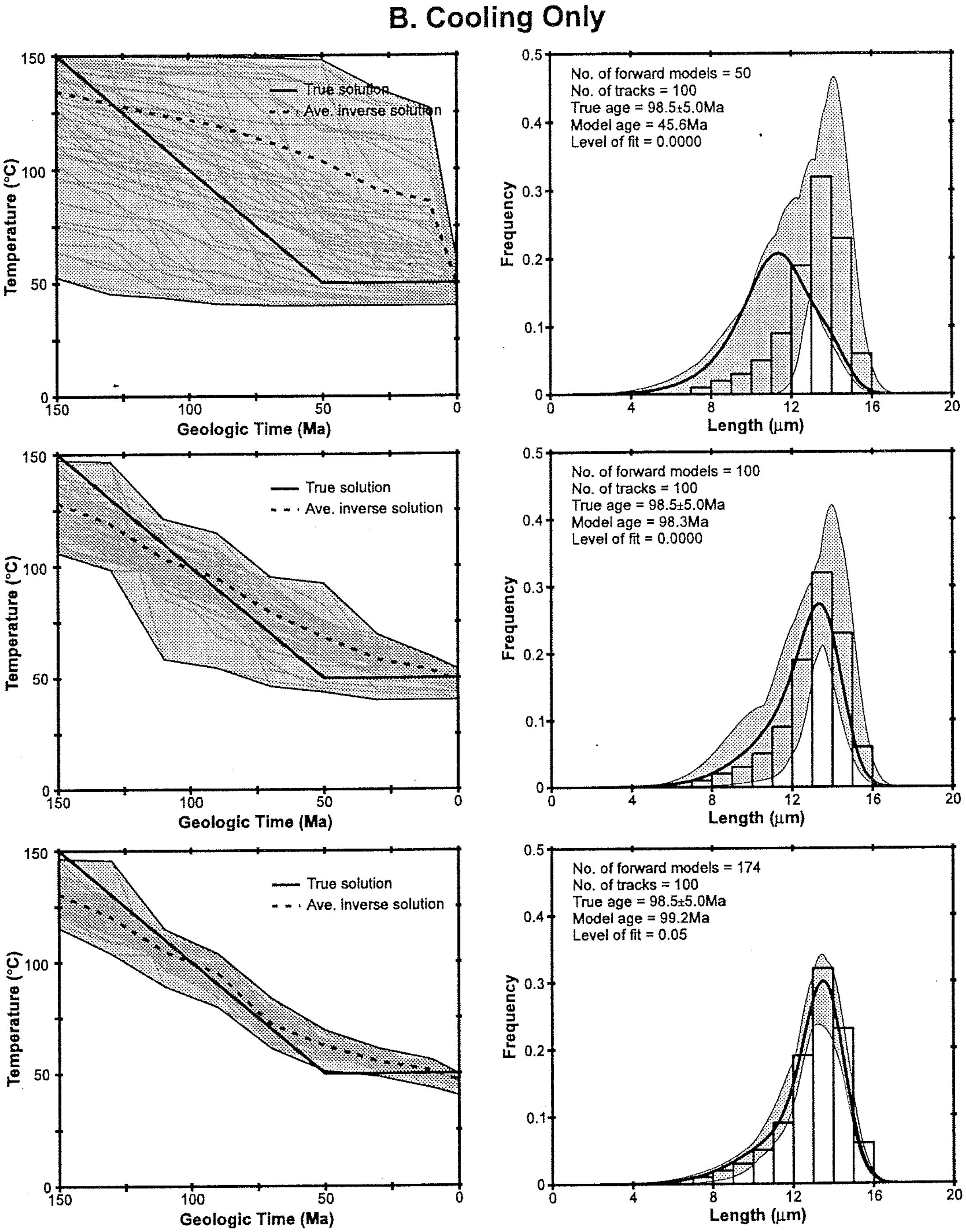


Figure 1. Continued.

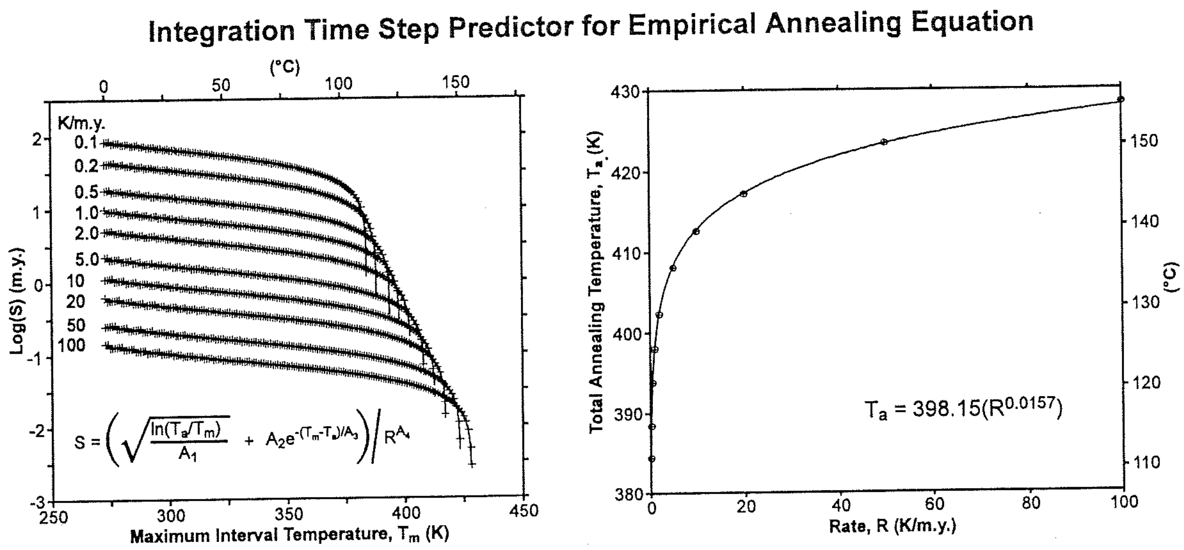


Figure 2. Left panel shows isothermal time step size predictor function (Issler, 1996) used for efficient and accurate evaluation of the empirical apatite fission track annealing equation. Step size (S) is a function of heating/cooling rate as well as the maximum interval temperature. Annealing calculations can be specified to an approximate level of accuracy by scaling S values by the factor $(10E)^{1/2}$ where E is the approximate percentage error on calculated track lengths (default is 0.1% accuracy). The crosses represent numerical data for the Crowley *et al.* (1991) Durango model, at the 0.1% accuracy level, which was used to fit the equation for S (solid curves). The right panel shows how the total annealing temperature, T_a, varies as a function of the rate of temperature change, R. T_a is defined as the temperature at which calculated track lengths become effectively 0.

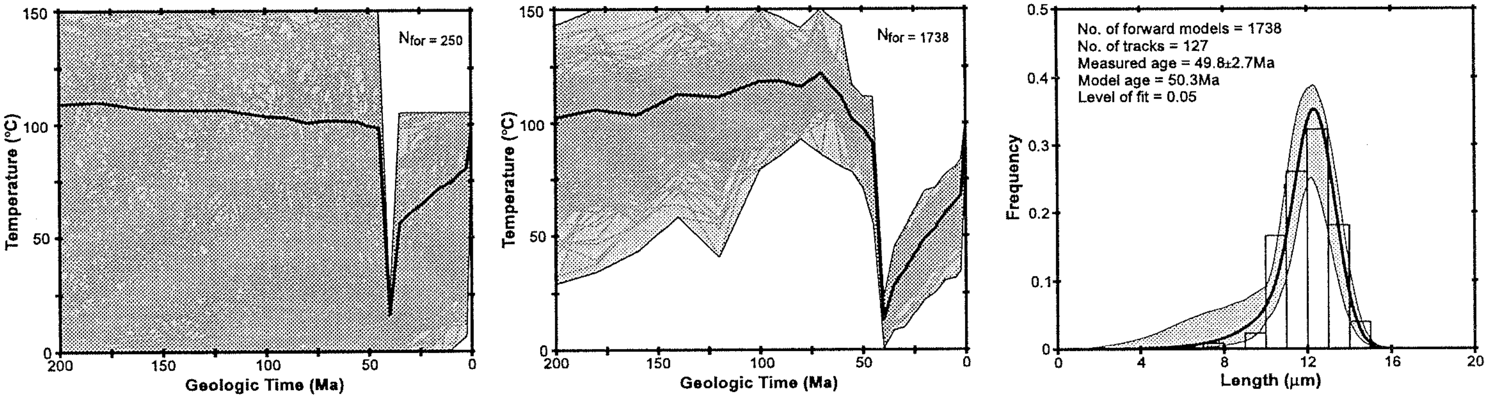
rate limiting step because, for certain temperature ranges, the program is prevented from using the much larger isothermal steps provided by the step size predictor function. Furthermore, as DELSUB decreases, the number of model iterations increases with increasing number of substeps for a given thermal history. If DELSUB is increased to 10 m.y., iterations decrease significantly and larger isothermal step sizes can be taken. This could lead up to a 10x increase in model speed. Nevertheless, there are situations where a small value for DELSUB is warranted (young fission track ages) and making DELSUB too large will degrade model resolution and violate important assumptions on which the track component concept is based. To choose DELSUB, one should consider the fission track age and the number of components needed to ensure a smooth track length distribution. As the fission track age and model times increase, DELSUB can also be increased. The value of ACUR also affects model run time but the difference in run time between using the 0.1% and 1% accuracy level is not that great. An ACUR of 0.1% produces tracks that are ≤0.2% too long (≤0.2°C error in temperature) whereas an ACUR of 1% produces tracks that are ≤2% too long (≤1°C error).

Another modification concerns the generation of random thermal histories. Previously, TINV52 selected randomly for temperature at each model time step. This version selects randomly for rate of temperature change (random selection of projection angle between temperatures at adjacent time steps - a tangent function relationship) and uses it to calculate temperatures for the next time step (Figure 3). This process is repeated randomly in the forward and backward directions in order to build up a family of random thermal solutions. The general philosophy is that geological temperature changes are governed by rate-controlled geological processes (i.e. exhumation/burial, hydrothermal heating, cooling of an intrusion, mantle/lithospheric dynamics). This alternative formulation prevents the biasing of solutions towards extremal values (as in the case of random temperature selection) and it eliminates clustering of thermal histories (Figure 3). The resulting solutions look more random, average solutions are smoother and the model runs faster. Also, a modification was made to reduce the effects of temperature bounds on random temperature history generation. The model is first required to randomly heat or cool and then the random number is used to select the rate. This allows temperatures the possibility of travelling along a boundary rather than being forced to heat or cool when in close proximity to a boundary.

Another major modification to the original inverse model is the option for specifying the number of randomly generated heating/cooling events over a selected time range. The user can incorporate geological constraints into the model as in the earlier version (e.g. near surface temperatures at time of

Random Temperature History Generation

A. Random selection by rate of temperature change and correction for boundary effects



B. Random selection by temperature

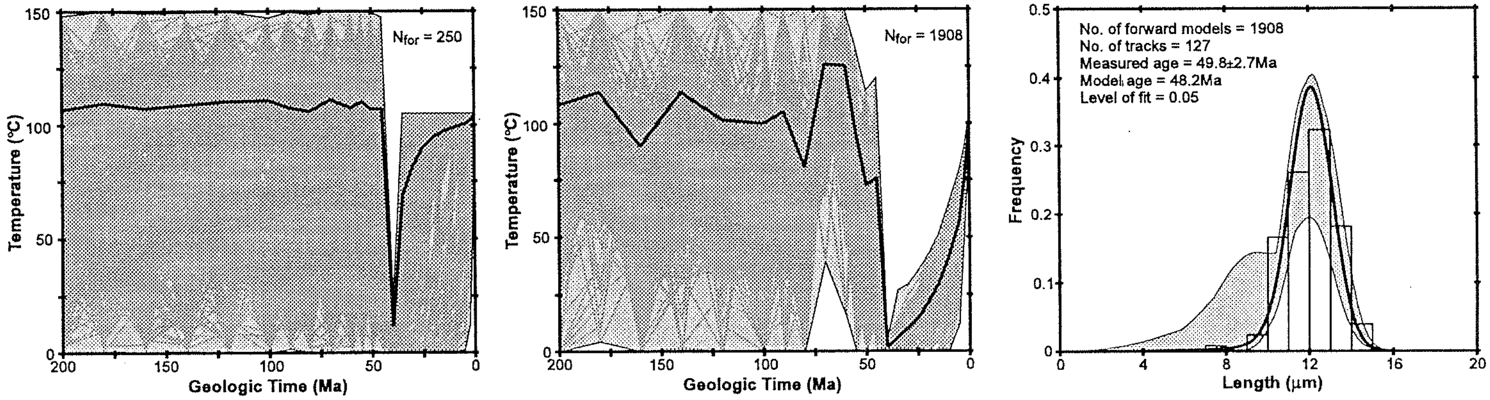


Figure 3. (A) Method of random temperature generation used in AFTINV32 and (B) method used in TINV52. Temperatures are generated randomly in the forward and reverse directions using (A) a random selection for rate of temperature change (tangent function of the projection angle between the new and previous point) and (B) a random selection between minimum and maximum temperature limits. For (A), an additional requirement is that the probability of heating or cooling is equal near a temperature boundary to minimize the effect of the imposed temperature limits. In comparison with A, method B is biased to higher rates of temperature change, with large cyclic flucuations yielding a wider range on parameter space for heating/cooling histories. However, for uni-directional temperature changes, method A tends to yield a wider range on acceptable parameter space.

deposition or the development of an unconformity, present temperatures, directions of temperature change, rates of temperature change typical of certain geological environments, temporal/thermal constraints from independent thermochronological data) and select time ranges over which rate bounds can be modified. Options on rate bounds include: 1) purely random heating/cooling; 2) monotonic heating or cooling during specific time ranges; and, 3) a specified number of thermal (heating or cooling) events (Figure 4). An example for the use of option 3 might be a simple foreland basin setting characterized by a single phase of burial and heating followed by exhumation and cooling. Selecting option 3 with one randomly generated heating event provides ranges for both time and maximum temperature that are permitted by the data. For option 3, the model randomly generates and filters solutions that have a specified number of heating/cooling events until it builds up a final set of statistically acceptable solutions. The model uses the user input temperature limits to select time ranges (these can be modified) over which rate limits can be customized. It uses cusps in the temperature envelope as natural break points.

AFTINV32 reads input from AFTMOD.BIN (output from PREAFT32). Output from AFTINV32 is written to the file, INFO (this contains many of the parameters written to PREAFT.OUT but includes model run time). Also, INFO contains descriptive information that is passed onto the program POSTFT32 (see Appendix III for example file). Calculated ages, lengths and temperature histories are written to the following binary files:

Default	Optional (not recommended)
(0.05 significance level)	(0.5 significance level)
TINV.S05	TINV.SOL

TINV.S05 contains the following information:

- age data for exponential mean thermal (preferred) solution
- temperature data for all statistically acceptable solutions

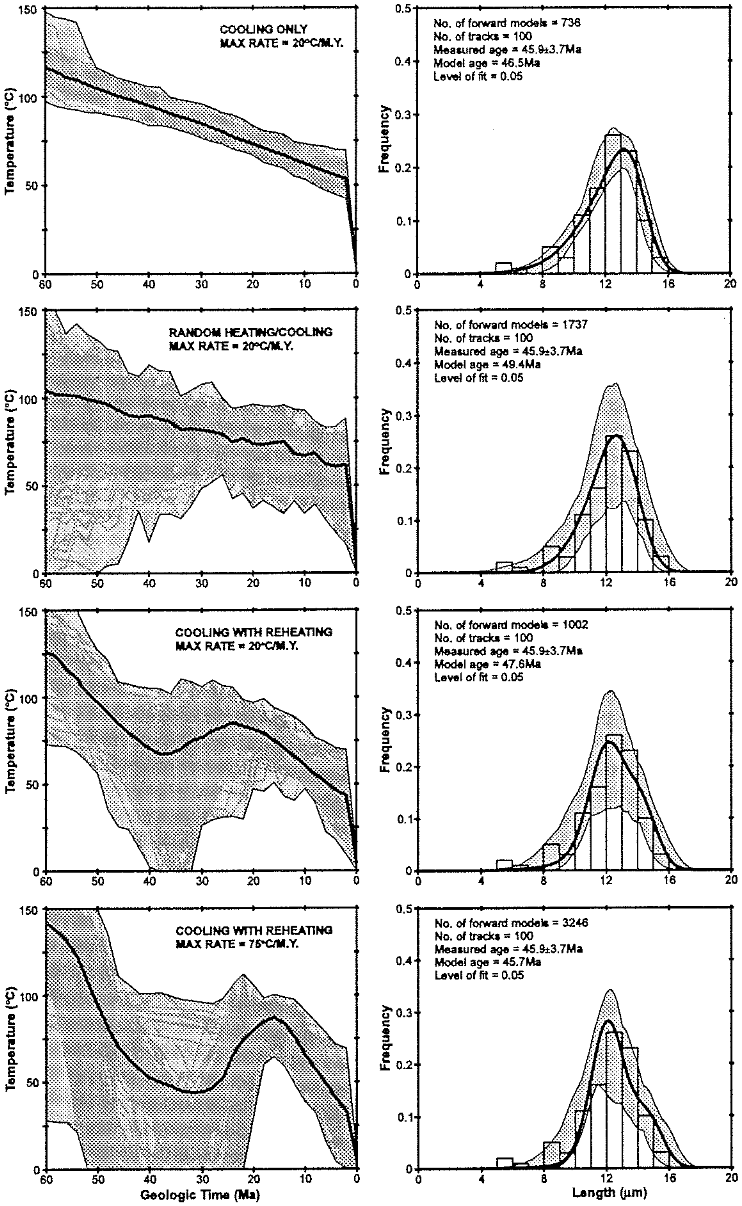


Figure 4. Illustration of different rate options for random temperature history generation. AFT sample is from a Tertiary granite in the internal zone of the southern Canadian Rocky Mountains (Omineca Belt). Wide open temperature limits (0-150°C) were used for all model times except for the present (0-10°C). For three of the models, heating/cooling rates were restricted to a maximum of 20°C/m.y., a reasonable maximum upper limit for burial/erosional processes typical of this tectonic setting. For the fourth model, maximum heating/cooling rates were determined by the initial temperature limits and model times (2 m.y. steps). The cooling only model shows a steady monotonic decrease in temperature with an increase in cooling rate in the last 2 million years. The recent cooling may be an artifact of the annealing model which has poor resolution at lower temperatures. Similar results are obtained for the random heating/cooling model (compare mean solutions (bold curve)). The last two models allow for a random reheating event. When rate limits are relaxed (lowermost panel), the model produces solutions indicating mild reheating (~85°C) during the Miocene. Although these solutions are nonunique, it is interesting that nearby samples from the southern Rocky Mountain Trench have Miocene ages and hydrothermal resetting is suspected.

- track length probability density function (PDF) for exponential mean solution (preferred solution)
- temperature data for minimum objective function solution of the retained solution set
- temperature data for exponential mean solution

TINV.SOL is used for intermediate file output, for solutions at the 0.5 level of significance and when the program fails to converge, at the 0.05 level. Allowing solutions to continue to the 0.5 level is not recommended because it increases dramatically model run time and doesn't add anything significant (This feature was added originally to obtain smoother looking average solutions but is unnecessary for the modified inverse model). TINV.S05 should be saved if future plotting of model results is required. POSTFT32 and the batch routine, GOFTPLT, will generate plots using the model results stored on this file. I recommend saving this file (along with INFO if you need to regenerate POSTAFT.OUT) under a different subdirectory and keeping the same default file names or things will get very confusing. The alternative is to just rerun the model and recreate the same solution if needed in the future. It is not necessary to store the plot files because they can be regenerated easily using the batch routine, GOFTPLT.

POSTFT32 This is an interactive FORTRAN program for post-processing model results stored on the binary file, TINV.S05 (output from AFTINV32). The program can be run by executing the batch file GOFTPLT. The user can specify plot parameters and the program generates formatted plot files with the .PL extension. Model results are written to POSTAFT.OUT (This is the output file you want because it contains all the significant results from the inverse model; see Appendix III). Six formatted plot files are generated by

POSTFT32:

0.05 significance level (default)	0.5 level (optional)
PDF05.PL	PDF5.PL
AVETMP05.PL	AVETMP5.PL
ALLTMP05.PL	ALLTMP5.PL
MINTMP05.PL	MINTMP5.PL
CLOSAG05.PL	CLOSAG5.PL
ALLPDF05.PL	ALLPDF5.PL

The .PL files are formatted plot files which require further processing by the following 16-bit FORTRAN executables to generate screen graphics and hard copy output using calls to the plotting routines of PLOT88. ZPVIEW generates screen plots, ZPLOT is used to make DXF format plot files which can be imported into graphics packages like CorelDraw, and ZPPOST generates postscript format plot files for copying to a printer. These are modified versions of ZPLOT which was written by Ross Boutilier of the GSC in Dartmouth, Nova Scotia. Default plot dimensions are stored in the file AFTPLOT.PAR (see Appendix II) which can be overwritten during execution of POSTFT32. Users can customize GOFTPLT to eliminate some of these plots.

ZPLOT Program which converts .PL files to DXF files. Other variations of this program are ZPVIEW (screen graphics) and ZPPOST (Postscript plot files). These programs use the .PL files as input and generate plots using calls to the PLOT88 graphics libraries. The batch file GOFTPLT executes POSTFT32 (generates .PL files) and ZPLOT and its variants to produce six plot files (see Appendix IV for examples). These are:

AVET.DXF, .PS - mean temperature (preferred) solution
MINT.DXF, .PS - minimum objective solution
\- best fit solution in the final set but not the optimum solution in a global sense
ALLT.DXF, .PS - retained solution set containing NSEAR statistically

acceptable model thermal histories

PDF.DXF, .PS - theoretical track length distribution or probability density function (PDF) for the mean temperature solution plus the bounding envelopes calculated for the retained solution set

ALLPDF.DXF, .PS - contains all PDF's for the retained solution set

CLOS.DXF, .PS - model closure age distributions for all thermal solutions

The model closure age represents the age of the oldest non-zero length track and it is dependent on the accuracy of the annealing model at high degrees of annealing (see Appendix III). These ages are controversial because annealing models are poorly constrained by experimental data at high degrees of track annealing where tracks become difficult to observe. When normalized mean track length (reduced length/initial length) drops below approximately 0.4, fission track ages go to zero and tracks are no longer visible (Green, 1988).

DXF files can be imported into CORELDRAW for viewing, modifying and printing. Once again, it is advisable to use the default names for all output files but to keep them in separate sample subdirectories. There are a lot of files and it can get confusing if sample names are used to rename plot and output files, especially when multiple runs are undertaken for the same sample.

RUNNING THE INVERSE MODEL

Below are instructions for executing the sequence of programs that comprise the inverse model. There are 4 major components to the inverse modelling procedure: data preparation, model initialization, model execution, and processing and plotting of model output. Relevant portions of screen output generated by the various programs (uppercase letters) are shown to illustrate the basic modelling steps. The programs can be run under the Windows 95 DOS window but significant improvements in model speed are achieved if the programs.are executed directly under Windows Explorer, especially if the I/O window is minimized during program execution.

1) **Data Preparation:** Prepare **sorted** track length files by executing **TSORT32** if this hasn't been done already. Either copy appropriate data files to the default file name (TRACK.IN) or enter the desired file name at the program prompt during execution (see below). Be sure that your track length data follow the same format as given in TRACK.IN (see Appendix II). The format is that used by the Dalhousie University Fission Track Research Laboratory. It consists of 9 lines of descriptive information (these are not used so you can enter 9 blank lines) followed by a line containing the total number of measured lengths. Below this, each line contains 2 pairs of numbers - the angle of the measured track with respect to the c-axis (first) and the measured length (second). The first parameter is not used by the current version of AFTINV32 so dummy values can be entered. However, future modifications to AFTINV32 will incorporate track orientation so it is a good idea to include measurements with respect to the c-axis. The data are read in using free format so a space or comma between numbers will suffice to delimit the values.

Just type and enter TSORT32 (if working within the DOS window) or "double click" on the executable file TSORT32 (within Windows 95 Explorer) to run the program and a window will come up displaying prompts concerning the file names to be used.

Step 1. Modify input/output/data file names as appropriate.

1. UNSORTED TRACK FILE	DATA\TRACK.IN
2. SORTED TRACK FILE	DATA\TRACK.SRT
3. OUTPUT FILE OF MODIFICATIONS	OUTPUT\TRACK.OUT

```
CHOOSE NUMBER TO MODIFY (RETURN TO CONTINUE)
```

Step 2. Enter sample fission track age plus one standard deviation. This information gets appended to the sorted track length file. (Remember to add one standard deviation because the default fitting of model ages is to within 2 standard deviations of the measured age - see discussion of parameter ASIG in Appendix I)

```
ENTER FISSION TRACK AGE AND ONE SIGMA (AGE,SIGMA)
```

Step 3. Hit return to close the window.

```
PROGRAM ENDED SUCCESSFULLY
HIT RETURN TO CLOSE WINDOW
```

Default file structures:

Input (default name):	Program:	Output (default names):
DATA\TRACK.IN	TSORT32	DATA\TRACK.SRT OUTPUT\TRACK.OUT

2) **Model Initialization:** Run **PREAFT32** (interactive program) to set up an inverse model run. It is a good idea to preview files INPUT\AFTSPL.IN and INPUT\AFTPARM.IN (Appendix II) to learn about the various model parameters. These files contain short descriptions of the parameters contained on them (also see Appendix I). They can be directly edited (be careful not to change the format or they can't be read by PREAFT32!) or they can be modified and overwritten during execution of PREAFT32 (the preferred, safer way except that entry of model times can be tedious). You might want to make and rename copies of these files in case they are accidentally altered. I recommend that the changes made to AFTSPL.IN are saved on different file names so that you can customize model setup parameters for certain data sets without having to keep recreating the same model parameters every time. For example, certain samples may be modelled with the same number of time steps so the information on AFTSPL.IN could be copied to a file with a different name.

Type and enter PREAFT32 (in DOS window) or “double click” on PREAFT32 (Windows 95 Explorer) and a window will appear containing screen I/O.

Step 1. Enter the appropriate file names or return for default if the appropriate information has already been copied to these files.

```
1. MODEL PARAMETER FILE        INPUT\AFTPARM.IN
2. SAMPLE PARAMETER FILE       INPUT\AFTSPL.IN
3. PARAMETER LIST OUTPUT       OUTPUT\PREAFT.OUT
4. BINARY FILE FOR AFT MODEL   INPUT\AFTMOD.BIN
5. DEFAULT AGE/LENGTH FILE     DATA\TRACK.SRT
CHOOSE NUMBER TO MODIFY FILE NAME (RETURN TO CONTINUE)
```

Step 2. Stop model at 0.05 significance level (default).

```
SELECT CONVERGENCE CRITERION FOR INVERSE FISSION TRACK
MODEL (DEFAULT IS 1):
1. STOP MODEL AT .05 SIGNIFICANCE LEVEL
2. STOP MODEL AT 0.5 SIGNIFICANCE LEVEL
ENTER VALUE (RETURN TO CONTINUE)
```

Step 3. You can examine and change annealing model coefficients (normally hit return to bypass this if you are using the same set of coefficients each time). The model uses the Crowley *et al.* (1991) 6-parameter annealing equation with optional coefficients for: Durango apatite, fluorapatite and Sr fluorapatite (Crowley *et al.*, 1991) and Durango apatite based on the 5-parameter equation of Laslett *et al.* (1987). Users also have the option to input their own set of coefficients.

```
DO YOU WISH TO REVIEW OR MODIFY TRACK LENGTH REDUCTION
MODEL COEFFICIENTS (Y OR N/RETURN)?
```

If yes is chosen, the following type of information appears.

```
1. CROWLEY ET AL ANNEALING MODEL FOR DURANGO APATITE
2. C1(1)  [C0]        = -0.320200E+01
3. C1(2)  [C1]        =  0.936700E-04
4. C1(3)  [-C2/C1]    = -0.196330E+02
5. C1(4)  [C3]        =  0.420000E-03
6. C1(5) [ALPHA]      =  0.490000E+00
7. C1(6) [BETA]       = 0.300000E+01

TIME STEP PREDICTOR COEFFICIENTS:
A(1) =  0.59600E-02
A(2) =  0.43000E-01
A(3) =  0.34800E+02
A(4) =  0.97800E+00
A(5) =  0.39815E+03
A(6) =  0.15700E-01
CHANGE ANNEALING MODEL COEFFICIENTS (Y OR N)?
```

If yes is selected, the screen displays the following options:

```
1. CROWLEY ET AL DURANGO APATITE
2. LASLETT ET AL DURANGO APATITE
3. CROWLEY ET AL FLUORAPATITE
4. CROWLEY ET AL SR FLUORAPATITE
5. ENTER NEW COEFFICIENTS
CHOOSE 1, 2, 3, 4 OR 5
```

If 1, 2 3, or 4 is chosen, the selected model coefficients are displayed as above. However, if option 5 is selected, the user is required to enter new model parameters for both the annealing model and the time step predictor function. The time step predictor function is normalized to the total annealing temperature, T_a, which is unique for each compositional annealing model. At the very least, users should determine the appropriate values for the equation predicting T_a as a function of the rate of temperature change (coefficients A(5) and A(6) above, see Figure 2 and Appendix V). If appropriate changes are not made to the time step predictor function, solutions to the annealing equation may not be accurate.

```
**CAUTION: MAKE SURE THAT YOU CHANGE MODEL TIME STEP
PREDICTOR COEFFICIENTS AS WELL**


1. New annealing model
2. C1(1) [C0]        = value
3. C1(2) [C1]        = value
4. C1(3) [-C2/C1]   = value
5. C1(4) [C3]        = value
6. C1(5) [ALPHA] = value
7. C1(6) [BETA}   = value
SELECT LINE NUMBER TO BE MODIFIED
```

After changing the annealing model coefficients, the user is prompted to change the time step predictor coefficients.

```
TIME STEP PREDICTOR COEFFICIENTS:
MINIMUM REQUIRED CHANGE IS THAT COEFFICIENTS A(5) & A(6)
YIELD THE CORRECT TA
1. A(1) = value
2. A(2) = value
3. A(3) = value
4. A(4) = value
5. A(5) = value
6. A(6) = value
CHOOSE LINE TO MODIFY/RETURN TO CONTINUE
```

Step 4. Normally, you would say yes to reviewing/modifying model parameters. Modify sample parameters as needed (e.g. title information, sample name, date, model #, etc.). At this stage, if you want, you can change the random number generator seed value (iseed) or select one of 3 different random number generators (igen = 0, system; igen = 1 or 3 (Ran1 or Ran 3 from Press *et al.*, 1986)). Many of these parameters, which are read from AFTPARM.IN, don't have to be changed but the option is available to do so. Check AFTSPL.IN and AFTPARM.IN for descriptions of these and other parameters.

```
TEMPERATURE LIMIT AND RATE BOUND CHECK COMPLETE
DO YOU WISH TO REVIEW OR MODIFY MODEL PARAMETERS?
TYPE Y (YES) OR N (NO)
```

If yes is chosen, the following screen display appears.

```
1.  Sample title information
2. Model run information
3. DELSUB    = value
4. ACUR      = 0.100
5. IGEN      = 0
6. ISEED     = value
7. MAXFOR    = 25000
8. NOUT      = 50
9. NSEAR     = 250
CHOOSE NUMBER TO MODIFY (RETURN TO CONTINUE)
```

Step 5. The next step involves choosing the model times. Geologic time is assumed as the default.

```
YOU MAY EXPRESS TIME AS GEOLOGIC TIME (MA) OR MODEL TIME
(MYR; I.E. T = 0 MYR AT START):
MA (0) OR MYR (1), IMOD = 0
MODIFY? (Y OR N OR RETURN TO CONTINUE)
```

Step 6. Select the number of model time points.

```
NUMBER OF TIME POINTS, M1 = value
MODEL TIMES:
 1 value
 2 value
   .
   .
   .
DO YOU WANT TO CHANGE THE TOTAL NUMBER OF TIME POINTS
(M1) (Y OR N/RETURN)?
```

Step 7. Change values in time array if necessary.

```
MODEL TIMES:
 1 value
 2 value
   .
   .
   .
DO YOU WANT TO CHANGE TIME VALUES (Y OR N/RETURN)?
```

Step 8. Set temperature limits. Choose upper and lower temperature ranges for corresponding model times. Incorporate available temperature constraints but don't overconstrain the model by choosing narrow temperature ranges without supporting data. I choose 0°C and 150°C as the lower and upper temperature limit, respectively, when temperatures are totally unconstrained.

```
LOWER AND UPPER TEMPERATURE LIMITS:
    TLOW    TUP     TIME
 1  value   value   value
 2   .       .       .
     .       .       .
```

```
DO YOU WANT TO CHANGE VALUES? (Y OR N/RETURN)
```

Step 9. Select temperature rate constraints corresponding to time-temperature limits using either:

1. Use previously calculated rates stored on file or generated on first pass through the program (default).

or

2. Use maximum rates calculated from the user-specified temperature limits.

(**Note: Rate constraints are purposely separated from temperature limits because users may want to limit the rate of temperature change to values that are characteristic for certain geological settings. This added flexibility also complicates temperature/rate bound setup and increases the possibility that something may go wrong. Logic checking is imbedded in the code to warn users of inconsistencies.)

```
SELECTION OF HEATING/COOLING RATE BOUNDS:
**CHOOSE OPTION 2 ON FIRST PASS IF YOU HAVE CHANGED MODEL
TIMES**
1. USE RATES FROM SAMPLE INPUT FILE OR CURRENT ARRAY
VALUES (ON MULTIPLE PASSES) (DEFAULT)
2. MIN/MAX RATES CALCULATED FROM INPUT TEMPERATURE LIMITS,
TLOW AND TUP
CHOOSE LINE NUMBER (RETURN FOR DEFAULT)
```

Step 10. Modify/customize the above rate limits (can change individual values or can select the time range for cooling or heating only or for constant heating or cooling). Be careful. If chosen rates prevent temperatures from staying within user-specified temperature limits, the program will tell you the offending line/s and not let you complete model set-up until the logic is sorted out.

```
RATE OF TEMPERATURE CHANGE PER TIME STEP:
(HRMAX, CRMAX MUST BE POSITIVE REAL NUMBERS)
```

```
HRMAX > CRMAX (HEATING>COOLING)
CRMAX > HRMAX (COOLING>HEATING)
CRMAX = HRMAX (COOLING=HEATING)
HRMAX = 0; CRMAX > 0 (COOLING ONLY)
CRMAX = 0; HRMAX > 0 (HEATING ONLY)
HIT RETURN TO CONTINUE
MAX RATES(DEG/MY) TIME INTERVAL TEMPERATURE LIMIT CHANGE
 HEATING  COOLING                      TLOW        TUP
  HRMAX    CRMAX
1 value    value     value - value   value-value   value-value
    .        .          .     .        .     .       .     .
    .        .          .     .        .     .       .     .
HIT RETURN TO CONTINUE
1. MODIFY AND CUSTOMIZE ABOVE RATE/TEMPERATURE BOUNDS
2. GO BACK AND REVIEW ABOVE LIMITS
CHOOSE LINE NUMBER (RETURN FOR NO CHANGES)
```

Option 2 sends you back to the beginning of step 10. If option 1 is selected, the following choices are available.

```
1. MODIFY INDIVIDUAL VALUES
2. SELECT TIME RANGE FOR COOLING ONLY
3. SELECT TIME RANGE FOR HEATING ONLY
4. SET HEATING RATES TO A SPECIFIED VALUE OVER A SELECTED
TIME RANGE
5. SET COOLING RATES TO A SPECIFIED VALUE OVER A SELECTED
TIME RANGE
CHOOSE LINE NUMBER (RETURN FOR NO CHANGES)
```

Step 11. Option to segment the thermal history into selected time ranges and to specify the number of thermal events. Be very careful here. In particular, diverging or converging temperature envelopes will cause problems if mono-directional temperature changes are selected (due to the logical incompatibility). Only the purely random heating/cooling condition will work under these circumstances (boundaries that slope the same direction are okay). The program contains some logic checking and will give warnings for poorly chosen model parameters. However, there is no guarantee it is foolproof. AFTINV32 is forced to stop if incorrectly chosen model parameters cause temperatures to exceed the specified temperature limits. On the first pass, the program will use parameters saved on AFTSPL.IN. These time ranges and rate constraints can be modified to suit the current model.

```
EXPRESS RATE BOUNDS IN TERMS OF THE NUMBER OF
PERMISSIBLE THERMAL EVENTS (RATES WILL BE ADJUSTED
DYNAMICALLY IN AFTINV32)

REGION  TIME RANGE        # OF EVENTS       NHP  NCP
                       HEATING  COOLING
  1     value-value    random   random       -1   -1
  2     value-value    no       monotonic     0   -1
  3     value-value    1        monotonic     1   -1

1. USE ABOVE VALUES (DEFAULT)
**OPTIONS 2 AND 3; PROGRAM SELECTS TIME RANGES OVER WHICH
THERMAL EVENTS ARE APPLIED. CUSPS IN t-T SPACE DEFINE
NATURAL BREAKS.**
2. USE UPPER T BOUNDS TO SELECT RANGE
3. USE LOWER T BOUNDS TO SELECT RANGE
4. OVERRIDE AUTOSELECT, CHOOSE CUSTOM RANGE/S
CHOOSE 1, 2, 3 OR 4, RETURN FOR DEFAULT
```

Following selection of one of the above options, the time ranges and rate constraints are listed again. If no changes were made, we have:

```
REGION   TIME RANGE          # OF EVENTS        NHP   NCP
                         HEATING   COOLING
  1      value-value     random    random        -1    -1
  2      value-value     no        monotonic      0    -1
  3      value-value     1         monotonic      1    -1
HIT RETURN TO CONTINUE
```

```
**CAUTION: CHOOSE PARAMETERS CAREFULLY!**
UNLIKE THE PURELY RANDOM HEATING/COOLING MODEL, CERTAIN
PARAMETER COMBINATIONS MAY CAUSE CALCULATED TIME-TEMP
POINTS TO EXCEED THE DEFINED SOLUTION DOMAIN. THE INVERSE
MODEL WILL TERMINATE IN THIS CASE. AVOID COMPLEX,
OVERCONSTRAINED TEMPERATURE BOUNDS WITH MANY SLOPING
BOUNDARIES WHEN SPECIFYING THE NUMBER OF THERMAL
EVENTS. IN PARTICULAR, AVOID DIVERGING/CONVERGING TEMP
BOUNDS WITH OPPOSITE DIRECTIONS OF CHANGE. SOLUTIONS ARE
BUILT IN FORWARD & REVERSE DIRECTIONS AND THIS WILL CAUSE
PROBLEMS WHEN ASSUMING UNI-DIRECTIONAL TEMPERATURE
CHANGES.

1. MODIFY HEATING/COOLING CONSTRAINTS?
2. MODIFY TIME RANGE/S?

CHOOSE 1 OR 2 (0 FOR NO CHANGES)
```

An additional series of options are available if 1 or 2 is chosen. For example, if option 1 is selected, the following screen display appears.

```
ENTER INDEX NO. FOR DESIRED TIME RANGE
```

After selecting the appropriate time range, the screen display changes to:

```
1. SELECT NUMBER OF HEATING PULSES (SUPERIMPOSED ON A
COOLING HISTORY)
2. SELECT NUMBER OF COOLING PULSES (SUPERIMPOSED ON A
HEATING HISTORY)
SELECT 1 OR 2/RETURN FOR NO CHANGES
```

If option 1 is chosen, we get:

```
IF NHP>0, NHP HEATING PULSES ARE SUPERIMPOSED ON A
COOLING ONLY HISTORY
IF NHP=0, COOLING ONLY HISTORY (***HEATING RATES RESET TO
0!***)
IF NHP=-1, RANDOM HEATING OR RANDOM MONOTONIC HEATING
WITH A COOLING EVENT/S

ENTER VALUE FOR NHP
```

Step 12. The program completes logic checking and if all is well, it asks if you want to review/modify model parameters. If no changes are necessary, continue to next stage (enter N for no).

```
TEMPERATURE LIMIT AND RATE BOUND CHECK COMPLETE
DO YOU WISH TO REVIEW OR MODIFY MODEL PARAMETERS?
TYPE Y (YES) OR N (NO)
```

Step 13. Option to overwrite changes on INPUT\AFTPARM.IN (generally few if any changes are made to this).

```
OVERWRITE PARAMETERS ON INPUT\AFTPARM.IN?
YES (Y) OR NO (N)/RETURN?
```

STEP 14. Option to overwrite changes on INPUT\AFTSPL.IN (or whatever file contains sample specific model information). If you made lots of changes and want to keep them, say yes. Otherwise, the changes will only exist on AFTMOD.BIN and will only apply to the current model run.

```
OVERWRITE PARAMETERS ON INPUT\AFTSPL.IN?
YES (Y) OR NO (N)/RETURN?
```

STEP 15. Hit return to close the window. (See Appendix III for example output)

```
PROGRAM FINISHED
HIT RETURN TO CLOSE WINDOW
```

Default file structures:

Input (default names):	Program:	Output (default names):
INPUT\AFTSPL.IN		
INPUT\AFTPARM.IN	PREAFT32	INPUT\AFTMOD.BIN
DATA\TRACK.SRT		OUTPUT\PREAFT.OUT

3) **Model Execution:** Run **AFTINV32**, the constrained random search inversion model. Model run times can be highly variable, depending on factors such as 1) the complexity of the time-temperature limits; 2) the value of parameters like DELSUB and ACUR; 3) the number of randomly generated thermal solutions defining the parameter search space (NSEAR); 4) the number of model time steps; 5) the type of options used for controlling the rate of temperature change and 6) the degree to which the model is constrained (tightly constrained models may have to work harder at finding acceptable solutions). Increasing the values of DELSUB and ACUR leads to a shorter model run time, but coarser model discretization and less accuracy. Typical run times can vary from on the order of minutes to an hour for a 486-66MHz PC but the model can take considerably longer to run if it has problems converging. In one example, the number of forward models required for convergence (>22,000) decreased by almost an order of magnitude (<3000) by slight modification of model parameters and choosing different rate options. Models on my Pentium 100 execute in a little less than 50% of the time that they took on my older 486-66MHz PC.

To run the inverse model, type and enter AFTINV32 (AFTINV32 will run at least 5% faster if run under Windows Explorer instead of under the DOS window - just "double click" on the executable file name). A window will open displaying the progress of model calculations. **Hint:** The model will run an additional ~5-10% faster if the window is minimized during program execution (click on horizontal bar (leftmost icon in upper right hand corner of window) to minimize the window; clicking on the x will shut down the program and close the window). As with all windowed applications under Windows 95, click on the program name on the horizontal bar at the bottom of the screen to restore the window. (See Appendix III for example output)

Default file structures:

Input (default binary file):	Program:	Output
INPUT\AFTMOD.BIN	AFTINV32	OUTPUT\INFO OUTPUT\TINV.S05 OUTPUT\TINV.SOL

4) **Processing and Plotting of Model Output:** Run **GOFTPLT** (executes POSTFT32, ZPLOT, ZPVIEW and ZPPOST) to prepare inverse model output and plot files.

Type and enter GOFTPLT or "double click" on GOFTPLT under Windows 95 Explorer to execute POSTFT32. A window opens displaying model input/output.

Step 1. Choose plotting of 0.05 significance level solutions (default - return).

```
PLOT OPTIONS:
1. PLOT .05 SIGNIFICANCE LEVEL SOLUTIONS ONLY (DEFAULT VALUE)
2. PLOT .05 AND .5 SIGNIFICANCE LEVEL SOLUTIONS
ENTER 1 OR 2 OR RETURN FOR DEFAULT
```

Step 2. Accept default plot file names (return).

```
MODEL PLOT FILES
1. TRACK LENGTH DISTRIBUTION (.05)    PLOT\PDF05.PL
2. AVE TEMPERATURE SOLUTION (.05)     PLOT\AVETMP05.PL
3. MINIMUM OBJECTIVE SOLUTION (.05)   PLOT\MINTMP05.PL
4. TEMPERATURE SOLUTION SET (.05)     PLOT\ALLTMP05.PL
5. CLOSURE AGE DISTRIBUTION (.05)     PLOT\CLOSAG05.PL
6. PDFS FOR ALL SOLUTIONS (.05)       PLOT\ALLPDF05.PL
CHOOSE NUMBER TO MODIFY (RETURN TO CONTINUE)
```

Step 3. Select output file name (return for default).

```
OUTPUT FILE FOR MODEL RESULTS    OUTPUT\POSTAFT.OUT
MODIFY FILE NAME? (Y/N OR RETURN TO CONTINUE)
```

Step 4. Choose yes if you wish to plot track lengths for all retained thermal solutions. This is necessary if you want to plot the envelope containing all acceptable track length solutions. If you choose yes, the program recalculates all the track lengths using the set of acceptable thermal solutions.

```
DO YOU WISH TO CALCULATE AND PLOT TRACK LENGTH
DISTRIBUTIONS FOR ALL THERMAL SOLUTIONS? (Y/RETURN OR N)
```

Step 5. Select yes if you want a plot title (return for no title). If yes is chosen, enter the plot title (maximum of 10 characters).

```
CHOOSE TITLE FOR PLOTS (MAX 10 CHARACTERS) (Y - YES; RETURN
FOR NO TITLE)
```

If yes is chosen, the following display appears.

```
ENTER PLOT TITLE
```

Enter title

```
PLOT TITLE IS title OK? (Y/N OR RETURN TO CONTINUE)
```

Step 6. Following the completion of track length calculations, the program asks if you want to:

1. Use saved plot parameters from AFTPLOT.PAR.
2. Let the program choose the plot dimensions using the input data.

```
PLOT SCALING AND LABELLING PARAMETERS
1. USE SAVED VALUES FROM FILE = INPUT\AFTPLOT.PAR
2. CALCULATE PLOT PARAMETERS USING INPUT DATA
IN BOTH CASES, PARAMETERS CAN BE MODIFIED LATER
CHOOSE 1 OR 2/RETURN FOR DEFAULT
```

Generally, it is better to select option 2 and let the program determine appropriate axes scaling and labelling. If you have specialized plot parameters already stored on AFTPLOT.PAR and wish to use them then select option 1.

Step 7. Review and modify plot parameters if necessary.

```
TEMPERATURE HISTORY PLOT PARAMETERS:
1. MAXIMUM TIME (MA) (X-AXIS), XTIMX = value
2. MAXIMUM TEMPERATURE (DEG C) (Y-AXIS), YTEMX = value
3. NO. OF TICK MARKS (X-AXIS), NDVTIMX = value
4. NO. OF TICK MARKS (Y-AXIS), NDVTEMY = value
ENTER LINE NUMBER TO MODIFY (RETURN TO CONTINUE)

MINIMUM CLOSURE AGE IS   value
MAXIMUM CLOSURE AGE IS value
MAXIMUM FREQUENCY VALUE IS value

CLOSURE AGE DISTRIBUTION PLOT PARAMETERS:
1. NO. OF AGE BINS, NBIN = value
(WHERE NBIN=(XAGEMX-XAGEMN)/DELBIN)
2. AGE BIN WIDTH (MA), DELBIN = value
```

```
3. MINIMUM AGE (X-AXIS), XAGEMN = value
4. MAXIMUM AGE (X-AXIS), XAGEMX = value
5. MAXIMUM FREQUENCY VALUE (0-1.0) ON Y-AXIS, YAGEMX = value
6. NO. OF TICK MARKS (X-AXIS), NDVAGEX = value
7. NO. OF TICK MARKS (Y-AXIS), NDVAGEY = value
8. NO. OF DECIMAL PLACES FOR Y-AXIS LABELS, NDCAGEY = value
CHOOSE LINE NUMBER TO MODIFY (RETURN TO CONTINUE)
```

Step 8. Option to overwrite plot parameters on AFTPLOT.PAR.

```
DO YOU WANT TO OVERWRITE NEW PLOT PARAMETERS ON FILE
AFTPLOT.PAR? (Y OR N OR RETURN TO CONTINUE)
```

Step 9. Hit return to exit window.

```
EXECUTED SUCCESSFULLY
HIT RETURN TO CLOSE WINDOW
```

Step 10. There is a pause exiting the window and returning to the DOS prompt. The pause was inserted deliberately in the batch routine after the execution of POSTFT32 to allow for the program window to close and the DOS window to open. If the pause is not present, the on screen plotting will not function correctly. Hit return to start generating plot files. A series of successive plots will appear on the monitor. Hit return twice (not too quickly) to clear each plot from the screen and initiate the next plot.

Step 11. If hard copies of the plots are desired, then copy the PLOT*.PS files to the printer. Alternatively, import the DXF versions of the plots into a drawing package such as CORELDRAW where they can be modified for slide, poster or manuscript preparation.

POSTFT32 prepares formatted plot files and lists model results:

Input:	Program:	Output:
OUTPUT\TINV.S05		OUTPUT\POSTAFT.OUT
OUTPUT\TINV.SOL		PLOT\AVETMP05.PL
OUTPUT\INFO		PLOT\MINTMP05.PL
OUTPUT\AFTPLOT.PAR	POSTFT32	PLOT\ALLTMP05.PL
		PLOT\CLOSAG05.PL
		PLOT\ALLPDF05.PL
		PLOT\PDF05.PL

ZPLOT converts .PL files to DXF files which can be imported into commercial packages such as CORELDRAW. ZPPOST creates Postscript plot files (.PS) that can be copied to a printer and ZPVIEW creates screen plots. Users should modify GOFTPLT if they do not want all of these plots. (see Appendix III for example output and Appendix IV for example plots)

Input:	Program:	Plots:
PLOT\AVETMP05.PL		PLOT\AVET.DXF, .PS
PLOT\MINTMP05.PL		PLOT\MINT.DXF, .PS
PLOT\ALLTMP05.PL	ZPLOT, ZPPOST	PLOT\ALLT.DXF, .PS
PLOT\CLOSAG05.PL		PLOT\CLOS.DXF, .PS
PLOT\ALLPDF05.PL		PLOT\ALLPDF.DXF, .PS
PLOT\PDF05.PL		PLOT\PDF.DXF, .PS

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APPENDIX I - MODEL PARAMETERS

The computer programs comprising the inverse model have been dimensioned to accept the following maximum values: 200 model time-temperature points, 2000 retained thermal solutions and 500 observed track lengths. These dimensions should be more than adequate for most situations.

This section contains a list of key model parameters, definitions and suggested values for these parameters. Users are encouraged to think carefully about selected model parameters and keep these in mind when interpreting model results. In a highly nonlinear model such as this, different parameter values may interact in complex ways to produce different results. It is good practice to run multiple simulations for the same samples using alternate parameters and look for common features in the resultant solutions. There are no general rules for deciding on the best parameter choices but users should be aware of how their choices affect model results.

Some of the options for parameters have not been tested and will need additional modifications in order to function properly. These are identified below and will be upgraded at a later date. They have been included to preserve some of Sean's initial code and to allow for incorporation of new advances in kinetic models for annealing.

A - Array of coefficients for the time step predictor function (Appendix V) used to solve the empirical apatite fission track annealing equation (6-parameter model) of Crowley *et al.* (1991). If annealing model coefficients, C1(1) to C1(6), are changed to reflect different apatite compositions, the corresponding A values must be changed as well or solutions to the annealing equation may be inaccurate.

ACUR - Parameter used with the model time step predictor function for integrating the fission track annealing equation. It gives the approximate numerical error for calculated track lengths and it affects the speed of model calculations. Values of 0.1 and 1.0 give reduced track length (r) values to ≤0.2% and ≤2.0%, respectively, of the "true" solution for a given thermal history. The corresponding errors in temperature are approximately ≤0.2°C and ≤1.0°C, respectively. The recommended default value for ACUR is 0.1.

ALPHA	- Expansion factor (set at 1.3). Used in the weighting of a random selection of temperatures from the thermal history set for the generation of new random thermal histories (part of the constrained search algorithm).
ASIG	- Number of standard deviations on the observed fission track age that is used for fitting calculated ages. Model fission track ages must lie within the observed age±ASIG standard deviations to be accepted. Normally, ASIG is 2 (**make sure that you enter one standard deviation on the sorted track length file because it gets multiplied by ASIG**).
CRMAX,HRMAX	- Arrays containing maximum allowable cooling and heating rates (°C/m.y.), respectively, that are used for the generation of random thermal histories. These values must be positive, real numbers that correspond to the time-temperature intervals set by the model time array and arrays TLOW and TUP. This option allows users to specify rates of change independently from the imposed temperature bounds. Users can either allow the program to calculate the rates using the values in TLOW, TUP and the model time array or they can customize the rates. When first setting up rates, it may be best to first calculate default rates and then modify them accordingly. Note that because rates can be decoupled from the temperature bounds, users may select inappropriate rate values that would prevent the model from staying within the specified temperature limits. When this happens, the program will issue a warning and identify the offending entries for examination and correction. Despite these potential problems, this option has many advantages. Users can control the direction (cooling

	- CRMAX>0 and HRMAX=0; heating - CRMAX=0 and HRMAX>0; both heating/cooling - CRMAX, HRMAX>0) and magnitude of random temperature change. For example, users may choose to restrict rates to values that may be characteristic for certain geological settings. If compelling geological evidence is available (e.g. continuous burial to present maximum temperatures, continuous exhumation), users may restrict parts of the thermal history to heating or cooling only. Users should choose rates carefully because they will have a major affect on the final acceptable range of parameter space. If rates are overconstrained, the range of acceptable solutions will be unrealistically narrow, implying a false level of precision in the results.
C1	- Array of 6 coefficients, C1(1) to C1(6), which correspond to the parameters, C_0, C_1, $-C_2/C_1$, C_3, α and β for the 6-parameter empirical annealing equation of Crowley *et al.* (1991). Model coefficients are given for the Crowley *et al.* (1991) fit to Durango apatite annealing data of Green *et al.* (1986), the Crowley *et al.* (1991) fluorapatite and Sr fluorapatite data and the Laslett *et al.* (1987) Durango apatite annealing model. User-supplied coefficients also are accepted by the inverse model.
C2	- Coefficients for the track component length variance function fit to the mean length versus standard deviation data of Green *et al.* (1986) using a cubic polynomial (Willet, 1992). This is necessary to model the broadening of observed mean track length distributions which accompanies increased annealing. Much of the spread in the data can be attributed to measuring tracks in all orientations with respect to the crystallographic c-axis (Donelick, 1991).
DELSUB	- Time for component track length generation (m.y.). Each component is assumed to be of constant age and behave similarly to single populations of induced tracks in annealing experiments. The final

track length distribution is calculated by combining all of the individual components. DELSUB is used to discretize model time intervals into an integer number of substeps. Therefore, it must be chosen as a real number which divides evenly into all model time intervals and it must not exceed the shortest model time interval. Program run time is sensitive to the value of DELSUB because it controls the number of substeps and can restrict the size of isothermal time step used by the program in the evaluation of the annealing model. Increasing its value will decrease model run time but possibly at the cost of decreased model resolution. DELSUB should be chosen to provide enough track components (at least 10-20) to ensure a smooth track length distribution. Therefore, DELSUB values of ≤5 m.y. may be appropriate for young samples (say ≤50 Ma) whereas a DELSUB of 10 m.y. may be suitable for older samples (say ≥200 Ma).

DELTA	- Reposition factor for the explicit temperature bounds (set to 0.001). Used to prevent randomly generated temperature histories, calculated from the retained set of random solutions, from straying outside of the initial user-defined temperature bounds.
IGEN	- Parameter for choosing the type of random number generator. For IGEN = 0, the model uses the function URAND of the Watcom F77 subprogram library to return pseudo-random numbers in the range (0.0,1.0). If IGEN = 1 or 3, the model uses the subroutines, RAN1 and RAN3, respectively, from Press *et al.* (1986). Subroutine RAN1 is based on the use of 3 linear congruential generators and RAN3 uses a subtractive method for random number generation.
IMOD	- When IMOD = 0, model times are expressed in terms of geologic time (Ma or m.y. before present) and model results and plots are presented this way. This is the default and the easiest, most intuitive way to set up a thermal history and interpret model results. For those

who see the world differently, there is an option to work in model time (m.y. after start of model) where time is initiated at 0 m.y. and progresses forward in time (IMOD=1). Whichever choice is made, the inverse model works in model time and displays results according to the value of IMOD.

INORM	- Parameter for selecting the type of objective function. This should be set for the Kolmogorov-Smirnov test (INORM=3). The Pearson chi-squared test (INORM=2) has been included as part of Sean's original code but has not been tested for the new version of the model.
ISEED	- ISEED can be any integer value and it is used to seed the random number generator.
MAXFOR	- Maximum number of forward model thermal histories permitted. The program will terminate if it hasn't converged before attaining MAXFOR solutions. Results will be written to TINV.SOL rather than TINV.S05. A suggested value is 25,000 but this value can be increased to whatever the user wants (with faster computers and a faster algorithm, the program can achieve 25,000 in a reasonable time). Normally, the model will converge in well under 10,000 forward models (typically ~5000 or less).
M1	- Number of model time points (M = M1-1 time steps) which can't exceed 200. The typical number of time points is likely between 10-30 and perhaps up to 50, depending on the sample age and the level of detail desired. Time points need not be spaced equally and model time intervals might vary between 1 and 10 m.y. for typical fission track samples but could be larger for old samples. For example, time spacing could be reduced where users desire increased resolution (such as during the later stages of the thermal history) and made wider where the thermal history is more poorly constrained (such as early in the sample history). It should be noted that the spacing of

time points will have an affect on allowable model heating/cooling rates. The minimum number of points needed to reproduce observed fission track parameters is not necessarily the best criterion to use, particularly for inverse models, because it automatically biases solutions to low rates of temperature change and will artificially restrict parameter space. This is because temperature is assumed to vary linearly between time points and fewer, more widely spaced times will severely restrict calculated rates of temperature change, resulting in a narrowly-defined, perhaps overly-optimistic region of acceptable solution space.

NAGE - Parameter for choosing the type of age reduction model. Set NAGE=1 for the empirical age reduction model based on the reduced track length versus reduced track density relation in Willett (1992) for the data of Green (1988). Age reduction linearly proportional to r (NAGE=2) is included to preserve Sean's initial code but is not recommended.

NHP,NCP - Arrays containing the number of imposed heating or cooling events, respectively, for a specified time interval. For the purposes of the program, a heating event is a period of temperature rise and a cooling event is a time interval over which temperature decreases. This is a flexible and powerful option which allows the program to randomly seek out times where temperature was at a maximum or when cooling could have occurred. It is different from the purely random model in that it searches selectively for specific families of solutions with a characteristic number of thermal events. For example, if it is reasonable to assume that maximum temperature was reached during a specific time period for a simple case of heating followed by cooling, the model will search for a range of acceptable peak temperatures and times at which they could have occurred. Note that certain values of NHP and NCP may override previous specifications in the arrays CRMAX and HRMAX. Users have the option of breaking the thermal history into sub-time intervals with different rate options. The program will automatically subdivide the time-temperature history using either the values of TUP or TLOW of the user-specified temperature limits. These time intervals can be modified or the user can create their own intervals. For each time interval, NHP and NCP options are displayed based on the values in CRMAX and HRMAX and these can be modified. When NHP=NCP=-1, the model allows for both random heating and cooling using the values in CRMAX and HRMAX. When NCP=0 (no cooling), there is random monotonic heating only. When NHP=0 (no heating), there is random monotonic cooling only. If either NHP or NCP is set to 0, corresponding values in either HRMAX or CRMAX are set to 0 if they weren't previously. For NCP>0 and NHP=-1, the model allows for NCP random cooling events (normally 1 if choosing this option) superimposed on an overall random monotonic heating history using the rates in CRMAX and HRMAX. Similarly, for NHP>0 and NCP=-1, the model allows for NHP random heating events (normally 1 if choosing this option) superimposed on an overall random monotonic cooling history. Users must choose their options carefully and insure that they are logically compatible with the temperature bounds. Warnings will be issued by the program if logic errors occur (e.g. using diverging/converging temperature limits with anything other than the random heating/cooling option). If errors get by the model setup program, PREAFT32, AFTINV32 will terminate when an error is detected. The maximum allowable number of sub-time intervals is 20 and rarely will more than 2 or 3 intervals be required for even the most complex temperature histories.

NOUT	- The largest value of the objective function is written to the file, INFO, for every NOUT forward models. It provides a record for the progress of model calculations. It is set at 50 but can be increased to reduce model output. The largest value of the objective function is written to the screen window for every forward model.
NSEAR	- Number of retained thermal solutions in parameter search space. Normally, ~250 solutions are adequate to characterize the acceptable parameter space but there are situations with complex temperature envelopes where more solutions may be needed. Increasing NSEAR significantly increases model run time because the model must replace a larger number of initial random thermal histories with statistically acceptable solutions, therefore requiring more model iterations.
NTYP	- Option for treatment of length data. The current version of AFTINV32 uses the conventional mean length (NTYP=1). Future versions of the code may allow for length correction with respect to the c-axis (NTYP=2) or the a-axis (NTYP=3) but are not currently operational.
RSTD	- Reduced length of age standard (0.9) used in the calculation of model fission track ages. This is used to account for the decreased mean length of age standards (~14.5μm) relative the assumed initial mean length (XL0) and is necessary for calculations to be consistent with the track length-track density relationship.
TLOW,TUP	- Arrays containing lower and upper temperature bounds for defining initial parameter search space. Each pair of values coincides with elements in the model time array. Values are expressed in degrees Celsius but absolute temperatures are used in the annealing model. These arrays can be used to incorporate any geological or present constraints on temperature at specific times. For example, narrow

limits can be placed on current temperatures for surface or subsurface (e.g. corrected bottomhole temperatures, DST temperatures) samples. Suitable near surface temperatures (say 0°-25°C) can be specified at the time of deposition of the sediment which contained the apatite sample or, for samples near unconformities, at the time of exposure to near surface temperatures. Other paleotemperature data (e.g. %Ro, CAI, TAI, Rock-Eval Tmax, fluid inclusion homogenization temperatures, etc.) may help to constrain TUP values. Typical maximum temperature ranges might extend from 0°C (TLOW) to 150°C (TUP) for an unconstrained segment of the thermal history. It is important that these temperature limits are carefully thought out because the model will look only for solutions that lie between these initial temperature limits and these initial bounds will be updated as the model proceeds. Users should not overconstrain the model by adding more complexity to the temperature bounds than is warranted by the data. Tightly constrained models may take longer to run or may require a larger number of retained solutions (larger value of NSEAR) to properly represent the acceptable solution space.

XL0,XL3E - Original unannealed track length, XL0, (16.15 μm) and initial mean radius of length ellipse, XL3E (set=0, not used in current version with NTYP=1).

APPENDIX II - EXAMPLE DATA AND MODEL PARAMETER FILES

This section contains unsorted and sorted track length data files (TRACK.IN, TRACK.SRT) and model parameter files (AFTSPL.IN, AFTPARM.IN, AFTPLOT.PAR) for an example of real apatite fission track data from a petroleum exploration well (Amerk O-09) in the offshore portion of the Beaufort-Mackenzie Basin of northern Canada. Note that these filenames are default names and can be changed. The core sample was obtained from Eocene age sediment (~40Ma) at a mean depth of 3824m (with respect to the seafloor) with an estimated present temperature (from corrected BHT's and DST temperatures) of 94°C. Fisson track measurements were performed by Sandy Grist (AMG) of the Dalhousie University Fission Track Research Laboratory as part of a contract with Amoco Canada. The sample has a mean length of 12.06±1.17μm and a fission track age of 49.8±2.7Ma (passed χ^2 test).

The raw data file containing 127 track lengths (TRACK.IN, p. 51-53) was processed using TSORT32 to generate the sorted file, TRACK.SRT (p. 54-55). The initial sample parameter file, AFTSPL.IN, was modified using the model set-up program, PREAFT32, and was overwritten with the new sample specific information (p. 56-57). Values on the model parameter file, AFTPARM.IN (p. 58), were left unmodified. Plot specific information is listed on the file, AFTPLOT.PAR (p. 59), which is read and can be modified during execution of the post-processing program, POSTFT32.

II.1 Example of an unsorted track length file - TRACK.IN

```
03/07/91
FT91-002
AMERK0-01 3860.5-3871
BEAUFORT SEA
A
AMG
FT LENGTH
µm
A
 127
 43.32602    13.34214
 72.57939    11.32118
 55.30653    12.22807
 80.55725    10.83104
 79.25285    10.89863
 89.31364    14.57423
 57.55498    14.00158
 51.65583    13.29938
 28.80490    13.36392
 46.76378    13.36337
 76.07267    12.45528
 76.06554    10.27952
 29.50749    11.42835
 69.67007    13.25905
 79.31212    13.12013
 75.97874    12.10076
 55.70683    10.61474
 67.23238    11.89247
 30.39343    13.83581
 31.78723    14.48131
 25.19749    11.67695
 50.37482    12.36858
 76.51845    12.13835
 79.77792    10.65576
 70.22260    12.06084
 22.38684    13.96622
 29.90091    10.74635
 27.15848    13.72978
 55.32556    12.03489
 27.99858    13.45879
 61.32973     7.31160
 79.35238    11.91731
 32.04435    12.45469
 15.29561    13.85751
 43.86607    10.68120
 49.22583    11.18311
 42.12269    12.68414
 53.87805    13.14836
 50.19965    13.23361
 44.53493    12.81379
 70.84084    11.70493
 48.11070    14.05892
 74.47202    13.47661
 54.18304    11.95650
 53.98828    12.79562
 20.28725    12.46306
 83.51855    12.99708
 36.99895    11.77924
 49.64056    11.96379
 44.25720    12.06385
 24.04750    13.78228
 64.08452    10.44696
```

54.72318	13.56462
51.18605	13.35956
60.28094	11.81847
19.86618	14.48566
71.33710	11.26172
50.07411	10.66394
60.22195	11.40032
43.13332	11.56474
62.32410	12.70476
41.09308	12.02360
70.74914	10.98523
83.20585	11.52654
52.17663	10.94501
61.85315	11.73161
47.26384	10.94213
60.70092	11.32096
38.58696	11.06371
44.54764	10.96867
73.25227	12.67229
51.27110	12.98365
44.64936	12.76889
22.07996	13.11884
37.11688	12.78482
65.93673	12.74685
64.11391	12.37348
61.47883	11.03630
84.70357	12.01857
56.14735	13.92434
48.88454	13.87988
71.38515	10.83685
68.57993	11.56915
77.88361	12.15372
42.67557	11.70493
74.17844	9.93055
86.51770	11.74318
87.13516	10.73258
35.64279	12.39383
44.92476	12.01070
85.79420	11.05407
53.87472	12.39383
49.36916	11.35602
59.06561	11.23695
74.77141	13.43698
87.86588	12.47627
31.30448	12.57688
72.33385	12.39266
68.94275	12.13116
55.90285	9.83663
88.67053	9.95614
46.92097	11.36562
73.89179	11.33359
69.69633	12.48327
43.35388	12.57688
49.06549	10.78687
48.81612	11.30297
66.19914	11.09063
40.88320	12.06887
84.43573	12.41161
52.75523	13.33323
66.13428	11.03740
60.07257	10.58112
37.40070	12.33011
35.02823	12.72573
47.23738	12.65354
58.18574	11.32332
74.90535	10.93614

29.06831	10.60469
84.26447	11.38224
40.13379	12.50557
52.72166	13.58783
88.43903	10.92728
65.75514	12.45606
65.58567	11.10635
31.93530	12.02098
61.60910	10.33829

II.2 Example of a sorted track length file - TRACK.SRT

```
127   49.8000000    2.7000000
.7311600E+01  .1000000E+01
.9836630E+01  .2000000E+01
.9930550E+01  .3000000E+01
.9956140E+01  .4000000E+01
.1027952E+02  .5000000E+01
.1033829E+02  .6000000E+01
.1044696E+02  .7000000E+01
.1058112E+02  .8000000E+01
.1060469E+02  .9000000E+01
.1061474E+02  .1000000E+02
.1065576E+02  .1100000E+02
.1066394E+02  .1200000E+02
.1068120E+02  .1300000E+02
.1073258E+02  .1400000E+02
.1074635E+02  .1500000E+02
.1078687E+02  .1600000E+02
.1083104E+02  .1700000E+02
.1083685E+02  .1800000E+02
.1089863E+02  .1900000E+02
.1092728E+02  .2000000E+02
.1093614E+02  .2100000E+02
.1094213E+02  .2200000E+02
.1094501E+02  .2300000E+02
.1096867E+02  .2400000E+02
.1098523E+02  .2500000E+02
.1103630E+02  .2600000E+02
.1103740E+02  .2700000E+02
.1105407E+02  .2800000E+02
.1106371E+02  .2900000E+02
.1109063E+02  .3000000E+02
.1110635E+02  .3100000E+02
.1118311E+02  .3200000E+02
.1123695E+02  .3300000E+02
.1126172E+02  .3400000E+02
.1130297E+02  .3500000E+02
.1132096E+02  .3600000E+02
.1132118E+02  .3700000E+02
.1132332E+02  .3800000E+02
.1133359E+02  .3900000E+02
.1135602E+02  .4000000E+02
.1136562E+02  .4100000E+02
.1138224E+02  .4200000E+02
.1140032E+02  .4300000E+02
.1142835E+02  .4400000E+02
.1152654E+02  .4500000E+02
.1156474E+02  .4600000E+02
.1156915E+02  .4700000E+02
.1167695E+02  .4800000E+02
.1170483E+02  .4900000E+02
.1170503E+02  .5000000E+02
.1173161E+02  .5100000E+02
.1174318E+02  .5200000E+02
.1177924E+02  .5300000E+02
.1181847E+02  .5400000E+02
.1189247E+02  .5500000E+02
.1191731E+02  .5600000E+02
.1195650E+02  .5700000E+02
.1196379E+02  .5800000E+02
.1201070E+02  .5900000E+02
.1201857E+02  .6000000E+02
.1202098E+02  .6100000E+02
.1202360E+02  .6200000E+02
```

```
.1203489E+02  .6300000E+02
.1206084E+02  .6400000E+02
.1206385E+02  .6500000E+02
.1206887E+02  .6600000E+02
.1210076E+02  .6700000E+02
.1213116E+02  .6800000E+02
.1213835E+02  .6900000E+02
.1215372E+02  .7000000E+02
.1222807E+02  .7100000E+02
.1233011E+02  .7200000E+02
.1236858E+02  .7300000E+02
.1237348E+02  .7400000E+02
.1239266E+02  .7500000E+02
.1239373E+02  .7600000E+02
.1239393E+02  .7700000E+02
.1241161E+02  .7800000E+02
.1245469E+02  .7900000E+02
.1245528E+02  .8000000E+02
.1245606E+02  .8100000E+02
.1246306E+02  .8200000E+02
.1247627E+02  .8300000E+02
.1248327E+02  .8400000E+02
.1250557E+02  .8500000E+02
.1257678E+02  .8600000E+02
.1257698E+02  .8700000E+02
.1265354E+02  .8800000E+02
.1267229E+02  .8900000E+02
.1268414E+02  .9000000E+02
.1270476E+02  .9100000E+02
.1272573E+02  .9200000E+02
.1274685E+02  .9300000E+02
.1276889E+02  .9400000E+02
.1278482E+02  .9500000E+02
.1279562E+02  .9600000E+02
.1281379E+02  .9700000E+02
.1298365E+02  .9800000E+02
.1299708E+02  .9900000E+02
.1311884E+02  .1000000E+03
.1312013E+02  .1010000E+03
.1314836E+02  .1020000E+03
.1323361E+02  .1030000E+03
.1325905E+02  .1040000E+03
.1329938E+02  .1050000E+03
.1333323E+02  .1060000E+03
.1334214E+02  .1070000E+03
.1335956E+02  .1080000E+03
.1336337E+02  .1090000E+03
.1336392E+02  .1100000E+03
.1343698E+02  .1110000E+03
.1345879E+02  .1120000E+03
.1347661E+02  .1130000E+03
.1356462E+02  .1140000E+03
.1358783E+02  .1150000E+03
.1372978E+02  .1160000E+03
.1378228E+02  .1170000E+03
.1383581E+02  .1180000E+03
.1385751E+02  .1190000E+03
.1387988E+02  .1200000E+03
.1392434E+02  .1210000E+03
.1396622E+02  .1220000E+03
.1400158E+02  .1230000E+03
.1405892E+02  .1240000E+03
.1448131E+02  .1250000E+03
.1448566E+02  .1260000E+03
.1457423E+02  .1270000E+03
```

II.3 Example model parameter file - AFTSPL.IN

```
* SAMPLE TITLE
AMERK O-09 3824mSFLR  Richards sequence (Eocene)
* MODEL RUN AND DATE
MODEL#1, RANDOM HEATING/COOLING & HEATING ONLY, SEP 27/96
* DELSUB - COMPONENT SUBSTEP LENGTH (MYR). CHOOSE A VALUE THAT DIVIDES
*              EVENLY INTO ALL SPECIFIED TIME INTERVALS.
 2.500
* M1 - NUMBER OF MODEL TIMES (***NOTE: NUMBER OF MODEL TIME STEPS
*        IS M = M1 - 1***)
 23
* IMOD - = 0, EXPRESS TIMES IN TERMS OF GEOLOGIC TIME (MA)
*           = 1, EXPRESS TIMES IN TERMS OF MODEL TIME (I.E. STARTS
*           AT 0 MYR)
 0
* LIST M1 TIMES
 200.00
 180.00
 160.00
 140.00
 120.00
 100.00
  90.00
  80.00
  70.00
  60.00
  55.00
  50.00
  45.00
  40.00
  35.00
  30.00
  25.00
  20.00
  15.00
  10.00
   5.00
   2.50
   0.00
* TEMPERATURE BOUNDS ON MODEL TIMES. INCLUDE AVAILABLE CONSTRAINTS
* (I.E. PRESENT TEMPERATURE RANGE, TEMPERATURE LIMITS AT DEPOSITION,
* ETC.). GIVE LOWER AND UPPER LIMITS FOR M1 MODEL TIMES.
* TLOW, TUP
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0   150.0
  0.0    25.0
  0.0   105.0
  0.0   105.0
  0.0   105.0
  0.0   105.0
  0.0   105.0
  0.0   105.0
  0.0   105.0
```

```
  0.0  105.0
 85.0  105.0
* LIMITS ON TEMPERATURE VARIATION PER MODEL TIME STEP.
* HRMAX - MAX HEATING RATE, CRMAX - MAX COOLING RATE; CRMAX, HRMAX>0
* (HEATING/COOLING); CRMAX>0, HRMAX=0 (COOLING); HRMAX>0, CRMAX=0 (HEATING)
* LIST M1 - 1 RATE BOUNDS (HRMAX, CRMAX) (MUST BE POSITIVE REAL NUMBERS)
  7.5    7.5
  7.5    7.5
  7.5    7.5
  7.5    7.5
  7.5    7.5
 15.0   15.0
 15.0   15.0
 15.0   15.0
 15.0   15.0
 30.0   30.0
 30.0   30.0
 30.0   30.0
  5.0   30.0
 21.0    0.0
 21.0    0.0
 21.0    0.0
 21.0    0.0
 21.0    0.0
 21.0    0.0
 21.0    0.0
 42.0    0.0
 42.0    0.0
* NUMBER OF TIME INTERVALS FOR SPECIFIED HEATING/COOLING EVENTS
  2
* INDEX NUMBERS OF ELEMENTS IN TIME ARRAY CORRESPONDING TO BOUNDARIES
* OF TIME RANGES FOR SPECIFIED HEATING/COOLING EVENTS
  1
 14
 23
* SPECIFIED NUMBER OF HEATING (NHP) AND COOLING (NCP) EVENTS FOR ABOVE
* CORRESPONDING TIME INTERVALS. NHP=NCP=-1 - RANDOM HEATING/COOLING AT
* ABOVE RATES; NHP=-1, NCP>0 - RANDOM MONOTONIC HEATING WITH NCP IMPOSED
* RANDOM COOLING EVENTS; NHP>0, NCP=-1 - RANDOM MONOTONIC COOLING WITH
* NHP IMPOSED RANDOM HEATING EVENTS; NHP = 0 - NO HEATING; NCP = 0, NO
* COOLING. (NHP,NCP)
 -1  -1
 -1   0
```

II.4 Example model parameter file - AFTPARM.IN

```
* NTYP - TREATMENT OF LENGTH DATA. 1 - CONVENTIONAL MEAN; 2 - CORRECTED
* TO C-AXIS ORIENTATION; 3 - CORRECTED TO A-AXIS ORIENTATION
 1
* XL0 - ORIGINAL TRACK LENGTH (MICRONS), XL3E - INITIAL MEAN RADIUS OF
* LENGTH ELLIPSE (NOT USED WHEN NTYP = 1)
 16.150    0.000
* IAN - TYPE OF ANNEALING MODEL
 1
* DESCRIBE TYPE OF ANNEALING MODEL
CROWLEY ET AL ANNEALING MODEL FOR DURANGO APATITE
* NC1 - NUMBER OF COEFFICIENTS FOR LENGTH REDUCTION FUNCTION
6
* ARRAY C1 - COEFFICIENTS FOR LENGTH REDUCTION FUNCTION LISTED IN ORDER
*          FROM 1 TO NC1
-0.320200E+01
 0.936700E-04
-0.196330E+02
 0.420000E-03
 0.490000E+00
 0.300000E+01
* ARRAY A - TIME STEP PREDICTOR COEFFICIENTS CORRESPONDING TO ANNEALING
* MODEL OF TYPE IAN (MUST BE 6 PARAMETERS)
 0.59600E-02
 0.43000E-01
 0.34800E+02
 0.97800E+00
 0.39815E+03
 0.15700E-01
* NC2 - NUMBER OF COEFFICIENTS FOR COMPONENT VARIANCE FUNCTION
 4
* ARRAY C2 - COEFFICIENTS FOR COMPONENT VARIANCE FUNCTION LISTED IN
*          ORDER FROM 1 TO NC2
 0.789900E+00
 0.303500E-02
-0.229830E-02
 0.000000E+00
* RSTD - REDUCED LENGTH OF AGE STANDARDS
0.900
* ASIG - NUMBER OF STANDARD DEVIATIONS FOR FITTING AGES
2.0
* ALPHA - EXPANSION FACTOR
1.300
* DELTA - REPOSITION FACTOR FOR EXPLICIT BOUND
0.0010
* MAXFOR - MAXIMUM NUMBER OF FORWARD MODEL CALCULATIONS PERMITTED
 25000
* NSEAR - NUMBER OF RETAINED SOLUTIONS IN PARAMETER SPACE
 250
* INORM - CHOICE OF OBJECTIVE FUNCTION: 2 - PEARSON CHI2;
*        3 - KOLMOGOROV-SMIRNOV
 3
* NOUT - OUTPUT LISTED EVERY NOUT FORWARD MODELS
 50
* ACUR - SPECIFIED NUMERICAL ERROR TOLERANCE (%) (SUGGEST DEFAULT OF 0.1%)
*     - USED IN INTEGRATION STEP SIZE FUNCTION (0.01 - HIGH ACCURACY)
 0.100
* NAGE - CHOICE OF AGE REDUCTION MODEL: 1 - EMPIRICAL; 2 - PROPORTIONAL
*       TO R
 1
* IGEN - SELECT RANDOM NUMBER GENERATOR: 0 - SYSTEM; 1 - RAN1; 3 - RAN3
 0
* ISEED - SEED FOR RANDOM NUMBER GENERATOR
 1958
```

II.5 Example plot parameter file - AFTPLOT.PAR

```
*PARAMETERS FOR PLOT FILES GENERATED BY PROGRAM POSTAFT
*TEMPERATURE HISTORY PLOTS:
*XTIMX - MAXIMUM TIME (MA) (X-AXIS)
 200.000
*XTIMN - MINIMUM TIME (MA) (X-AXIS)
   0.000
*YTEMX - MAXIMUM TEMPERATURE (DEG C) (Y-AXIS)
 150.000
*YTEMN - MINIMUM TEMPERATURE (DEG C) (Y-AXIS)
   0.000
*XTIMSTR - STARTING VALUE ON X-AXIS FOR LABELLING
 200.000
*XTIMSTP - STEP SIZE FOR X-AXIS LABELLING
 -25.000
*NDVTIMX - NUMBER OF TICK MARKS ON X-AXIS
  8
*YTEMSTR - STARTING VALUE ON Y-AXIS FOR LABELLING
   0.000
*YTEMSTP - STEP SIZE FOR Y-AXIS LABELLING
  25.000
*NDVTEMY - NUMBER OF TICK MARKS ON Y-AXIS
  6
*NDCTMY - NUMBER OF DECIMAL PLACES FOR Y-AXIS NUMBERS
  0
*PARAMETERS FOR CLOSURE AGE DISTRIBUTION PLOTS:
*NBIN - NUMBER OF AGE BINS
 30
*DELBIN - BIN WIDTH (MA)
   5.000
*XAGEMN - MINIMUM AGE (MA) (X-AXIS)
  50.000
*XAGEMX - MAXIMUM AGE (MA) (X-AXIS)
 200.000
*XAGESTR - STARTING VALUE FOR X-AXIS LABELLING
  50.000
*XAGESTP - STEP SIZE FOR X-AXIS LABELLING
  15.000
*NDVAGEX - NUMBER OF TICK MARKS ON X-AXIS
 10
*YAGEMN - MINIMUM FREQUENCY VALUE FOR Y-AXIS
   0.000
*YAGEMX - MAXIMUM FREQUENCY VALUE (0-1.0) FOR Y-AXIS
   0.500
*YAGESTR - STARTING VALUE FOR Y-AXIS LABELLING
   0.000
*YAGESTP - STEP SIZE FOR Y-AXIS LABELLING
   0.100
*NDVAGEY - NUMBER OF TICK MARKS ON Y-AXIS
  5
*NDCAGEY - NUMBER OF DECIMAL PLACES FOR Y-AXIS NUMBERS
  1
```

APPENDIX III - MODEL OUTPUT

Parameter files, AFTSPL.IN and AFTPARM.IN (see Appendix II), are read and can be modified during execution of PREAFT32, the set-up program for the inverse model. During execution of PREAFT32, model parameters are written to the binary file, AFTMOD.BIN, for use by the inverse model, AFTINV32, and relevant information is written to the file, PREAFT.OUT (p. 62-63), to provide a record of parameters used for a specific model run. For example, model temperature limits are wide open (0° to 150°C, p. 62) prior to deposition at 40Ma and, except for the last model time, are constrained loosely to be no greater than the estimated present temperature plus a conservative error of ~10°C after deposition (p.62-63). At the last model time, temperature limits are set at approximately the present temperature ±10°C. The maximum rate bounds were calculated using the temperature limits and corresponding model times, except after 40 Ma where the maximum cooling rate was set to 0 (CRMAX=0, p. 63) and the model was constrained to heat only. Geological information suggests that, after deposition, the sample effectively underwent continuous burial to temperatures that are probably a maximum today.

Parameter information and model run time is written to the file INFO (p. 64-65) during execution of AFTINV32. Much of the information is a repeat of what is contained on PREAFT.OUT. A summary of model constraints shows that purely random heating and cooling is permitted prior to 40 Ma but that only random heating is allowed after 40 Ma (p. 65). The model converged in approximately 10.2 minutes running on a 100 MHz Pentium clone after completing 1761 forward models. A similar model with a DELSUB of 5 (excluding the 2.5 Ma time step) ran in less than 1/3 of the time.

Model results were written to the binary file, TINV.S05, which is read by POSTFT32 during execution of the batch routine, GOFTPLT. Model results are listed in the file, POSTAFT.OUT (p. 66-69), which contains information from TINV.S05 and INFO. Temperature solutions are given for the exponential mean of all statistically acceptable solutions (in this case, 250) and for the solution with the lowest value for the objective function. The bounding values of temperature which envelope all acceptable solutions are also listed (p. 66). The mean solution is taken as the preferred solution. Also listed are the calculated fission track age, model closure age and value of the objective function for all 250 solutions (p. 66-68). The closure age is the age of the oldest non-zero length track. These ages are controversial and annealing model-dependent. They depend on the questionable assumption that the annealing model is accurate at extremely high degrees of annealing (where tracks approach 0 length) and they predict the time that the sample cools below the total annealing temperature (defined as temperature where the reduced track length, r, is nonzero).

The calculated fission track age of 51.1 Ma for the exponential mean (preferred) solution is in good agreement with the measured age of 49.8 Ma (p. 68). Results for the solution with the lowest value of the minimum objective function are shown also for comparison purposes. Although this may be the "best-fitting" solution of the retained set, it is certainly not the optimum solution in a global sense. The modelling approach taken here honours the fact that fission track data have limited precision and that a weighted average solution is more appropriate than attempting to search for the global minimum.

III.1 Example output from PREAFT32 - PREAFT.OUT

```
PREAFT32 VERSION 1.0; PROGRAMMER: DALE ISSLER
LAST MODIFIED: SEPT 26, 1996
32-BIT WATCOM F77 V.10.6 COMPILED FOR WINDOWS 95
GEOLOGICAL SURVEY OF CANADA, 3303-33RD ST. N.W.
CALGARY, AB, CANADA, T2L 2A7
PH: (403) 292-7172; FAX: (403) 292-7159
EMAIL: dissler@gsc.nrcan.gc.ca

AMERK O-09 3824mSFLR  Richards sequence (Eocene)

MODEL#1, RANDOM HEATING/COOLING & HEATING ONLY, SEP 27/96

CROWLEY ET AL ANNEALING MODEL FOR DURANGO APATITE


 INVERSION CONTROL PARAMETERS
 ---------------------------------------------
 MAXIMUM NUMBER OF FORWARD MODELS, MAXFOR =      25000
 INTERMEDIATE OUTPUT EVERY         50 FORWARD MODELS
 NUMBER OF SOLUTIONS (L), NSEAR =        250
 NUMERICAL ERROR (%), ACUR =      0.1000000
 KOL-SMIRNIV OBJ FN, INORM =          3
 NUMBER OF STANDARD DEVIATIONS TO FIT AGE: 2.0
 RANDOM NUMBER GENERATOR SEED, ISEED =        1958
 EXPANSION FACTOR (ALPHA) = 1.30
 REPOSITION FACTOR FOR EXPLICIT BOUND (DELTA) = 0.00
 ORIGINAL TRACK LENGTH (XL0) =  16.150
 CONVENTIONAL MEAN DATA
 EMPIRICAL MODEL OF AGE REDUCTION
 TRACK LENGTH REDUCTION COEFFICIENTS:
 -3.20199990  0.00009367 -19.63299942  0.00042000  0.49000001  3.00000000
 COMPONENT VARIANCE COEFFICIENTS:
  0.78990000  0.00303500  -0.00229830  0.00000000


 SAMPLE CONTROL PARAMETERS
 --------------------------------------------------
 COMPONENT SUBSTEP LENGTH (DELSUB) =  2.500 MYR
 NUMBER OF TIMESTEPS (M) =           22
 NUMBER OF PARAMETERS, M1 =           23

 MODEL TIMES EXPRESSED AS:

 GEOLOGIC TIME    MODEL TIME    TEMPERATURE BOUNDS (DEG C)
      MA             MYR              LOWER      UPPER
   200.000          0.000              0.0       150.0
   180.000         20.000              0.0       150.0
   160.000         40.000              0.0       150.0
   140.000         60.000              0.0       150.0
   120.000         80.000              0.0       150.0
   100.000        100.000              0.0       150.0
    90.000        110.000              0.0       150.0
    80.000        120.000              0.0       150.0
    70.000        130.000              0.0       150.0
    60.000        140.000              0.0       150.0
    55.000        145.000              0.0       150.0
    50.000        150.000              0.0       150.0
    45.000        155.000              0.0       150.0
    40.000        160.000              0.0        25.0
    35.000        165.000              0.0       105.0
    30.000        170.000              0.0       105.0
    25.000        175.000              0.0       105.0
    20.000        180.000              0.0       105.0
    15.000        185.000              0.0       105.0
```

```
   10.000            190.000            0.0       105.0
    5.000            195.000            0.0       105.0
    2.500            197.500            0.0       105.0
    0.000            200.000           85.0       105.0

MODEL TIME INTERVALS AND TEMPERATURE RATE BOUNDS:
TSTEP  # OF SUBSTEPS  HRMAX   CRMAX   TIME INTERVAL
  #        MSUB                           (MA)
  1          8          7.50    7.50   200.0 - 180.0
  2          8          7.50    7.50   180.0 - 160.0
  3          8          7.50    7.50   160.0 - 140.0
  4          8          7.50    7.50   140.0 - 120.0
  5          8          7.50    7.50   120.0 - 100.0
  6          4         15.00   15.00   100.0 -  90.0
  7          4         15.00   15.00    90.0 -  80.0
  8          4         15.00   15.00    80.0 -  70.0
  9          4         15.00   15.00    70.0 -  60.0
 10          2         30.00   30.00    60.0 -  55.0
 11          2         30.00   30.00    55.0 -  50.0
 12          2         30.00   30.00    50.0 -  45.0
 13          2          5.00   30.00    45.0 -  40.0
 14          2         21.00    0.00    40.0 -  35.0
 15          2         21.00    0.00    35.0 -  30.0
 16          2         21.00    0.00    30.0 -  25.0
 17          2         21.00    0.00    25.0 -  20.0
 18          2         21.00    0.00    20.0 -  15.0
 19          2         21.00    0.00    15.0 -  10.0
 20          2         21.00    0.00    10.0 -   5.0
 21          1         42.00    0.00     5.0 -   2.5
 22          1         42.00    0.00     2.5 -   0.0
```

III.2 Example output from AFTINV32 - INFO

```
month:        9 day:       27 year:      1996

start time:      11 h,       27 m,       52 s    .

AMERK O-09 3824mSFLR  Richards sequence (Eocene)
MODEL#1, RANDOM HEATING/COOLING & HEATING ONLY, SEP 27/96
CROWLEY ET AL ANNEALING MODEL FOR DURANGO APATITE

 AFTINV32 v. 1.0 (September 27, 1996)
 32-bit Watcom F77 v. 10.6 compiled for Windows 95
 as a Windows NT windowed executable
 code optimized for an Intel Pentium processor
 Original source code developed by Sean Willett
 Source code modified by Dale Issler


  inversion control parameters:
 ---------------------------------------------------
 number of solutions (l) =        250
 number of timesteps (m) =         22
 number of parameters (m+1) =          23
 NUMERICAL ACCURACY (%), ACUR =       0.1000000
 timestep length (delsub) =  2.500
 obj fnct (2 = chi2; 3 = kol-smirnov) =            3
 convergence tolerance (tol95) =       0.1206805
 convergence tolerance (toler) =       0.0739168
 number of standard deviations to fit age 2.0
 measured age  =  49.80
 sigma of error in measured age  =  2.70
 number of data (n) =          127
 number of tracks measured =          127
 intermediate output every           50 forward models
 random number generator seed =        1958
 system number generator urand(iseed)
 expansion factor (alpha) = 1.300
 reposition factor for explicit bound (delta) = 0.0010
 original track length (xl0) 16.150
 initial mean radius of length ellipse (xl3e) =  0.000
 conventional mean data
 empirical model of age reduction
 track length reduction coefs.:
-3.20199990   0.00009367 -19.63299942   0.00042000   0.49000001   3.00000000
 component variance coefs.:
  0.78990000   0.00303500  -0.00229830   0.00000000

    temperature bounds       rate bounds        delt
  1     0.00    150.00      7.50      7.50     20.00
  2     0.00    150.00      7.50      7.50     20.00
  3     0.00    150.00      7.50      7.50     20.00
  4     0.00    150.00      7.50      7.50     20.00
  5     0.00    150.00      7.50      7.50     20.00
  6     0.00    150.00     15.00     15.00     10.00
  7     0.00    150.00     15.00     15.00     10.00
  8     0.00    150.00     15.00     15.00     10.00
  9     0.00    150.00     15.00     15.00     10.00
 10     0.00    150.00     30.00     30.00      5.00
 11     0.00    150.00     30.00     30.00      5.00
 12     0.00    150.00     30.00     30.00      5.00
 13     0.00    150.00     30.00      5.00      5.00
 14     0.00     25.00      0.00     21.00      5.00
 15     0.00    105.00      0.00     21.00      5.00
 16     0.00    105.00      0.00     21.00      5.00
 17     0.00    105.00      0.00     21.00      5.00
```

```
18    0.00   105.00      0.00    21.00      5.00
19    0.00   105.00      0.00    21.00      5.00
20    0.00   105.00      0.00    21.00      5.00
21    0.00   105.00      0.00    42.00      2.50
22    0.00   105.00      0.00    42.00      2.50
23   85.00   105.00

HEATING/COOLING SELECTION SUMMARY:

REGION   TIME RANGE              # OF EVENTS            NHP    NCP
             MA               HEATING    COOLING
  1        200.0-  40.0        RANDOM    RANDOM          -1     -1
  2         40.0-   0.0      MONOTONIC     NO            -1      0

max obj function =      2.705997
max obj function =      2.606319
max obj function =      2.523945
max obj function =      2.388125
max obj function =      2.258172
max obj function =      1.987671
max obj function =      1.762427
max obj function =      1.616724
max obj function =      1.430217
max obj function =      1.272456
max obj function =      1.087770
max obj function =      0.960885
max obj function =      0.856131
max obj function =      0.763517
max obj function =      0.690689
max obj function =      0.546502
max obj function =      0.408451
max obj function =      0.340381
max obj function =      0.307326
max obj function =      0.280647
max obj function =      0.255871
max obj function =      0.225375
max obj function =      0.202898
max obj function =      0.188623
max obj function =      0.173389
max obj function =      0.161246
max obj function =      0.146234
max obj function =      0.137533
max obj function =      0.130351
max obj function =      0.122386
max obj function =      0.120645
CONVERGENCE AT 0.05 SIGNIFICANCE LEVEL
number of forward models:         1761
stop time:          11 h,         38 m,          5 s
stop date - month:          9 day:         27 year:        1996
total execution time =  0.170147 hours or   10.2088 minutes
```

III.3 Example output from POSTFT32 - POSTAFT.OUT

```
month:       9 day:       27 year:      1996

start time:     11 h,      27 m,      52 s

AMERK O-09 3824mSFLR  Richards sequence (Eocene)

MODEL#1, RANDOM HEATING/COOLING & HEATING ONLY, SEP 27/96

CROWLEY ET AL ANNEALING MODEL FOR DURANGO APATITE



 MODEL RESULTS AT .05 SIGNIFICANCE LEVEL
                    EXP MEAN        MIN OBJ       LOWER      UPPER
   TIME    TIME   TEMPERATURE    TEMPERATURE      TEMP       TEMP
   (MY)    (MA)     (DEG C)        (DEG C)        BOUND      BOUND
   0.00   200.00    103.00          111.60        18.72      150.00
  20.00   180.00    104.83           96.87        37.93      150.00
  40.00   160.00    105.24          105.56        46.40      146.50
  60.00   140.00    115.15          132.34        48.08      150.00
  80.00   120.00    114.92          133.95        59.16      150.00
 100.00   100.00    117.46          125.20        73.09      150.00
 110.00    90.00    116.88          112.09        84.32      150.00
 120.00    80.00    116.29          112.66        92.05      143.39
 130.00    70.00    124.60          142.18        91.73      150.00
 140.00    60.00    107.44          104.04        79.73      129.94
 145.00    55.00     99.81           89.59        66.19      119.71
 150.00    50.00     98.93           93.96        65.50      112.71
 155.00    45.00     91.71           84.74        54.74      114.06
 160.00    40.00     12.30            4.13         0.05       22.40
 165.00    35.00     27.13           17.37         6.64       44.87
 170.00    30.00     33.17           24.43         8.61       53.70
 175.00    25.00     42.11           34.12        16.71       62.69
 180.00    20.00     47.32           37.49        23.99       65.42
 185.00    15.00     53.02           45.40        28.39       71.86
 190.00    10.00     58.64           51.51        29.59       80.23
 195.00     5.00     64.62           65.46        35.84       81.89
 197.50     2.50     67.28           69.25        39.86       84.60
 200.00     0.00     94.75           96.78        86.54      101.78


        CALC     CLOSURE    OBJECTIVE        CALC     CLOSURE    OBJECTIVE
       FT AGE      AGE       FUNCTION       FT AGE      AGE       FUNCTION
        (MA)      (MA)                       (MA)      (MA)
   1   47.89      81.67     0.067728    2   54.99      90.00     0.116027
   3   52.92     175.00     0.106547    4   51.46      67.50     0.112896
   5   49.78      89.69     0.082005    6   54.33      75.00     0.101219
   7   47.42      91.67     0.080133    8   52.80      71.79     0.097706
   9   54.96     200.00     0.116197   10   49.54      75.00     0.076315
  11   51.56      73.75     0.101743   12   46.92     110.00     0.092856
  13   52.47      70.00     0.085935   14   44.65      60.90     0.115161
  15   51.42     107.50     0.097551   16   54.60      70.00     0.107218
  17   54.71      70.62     0.109708   18   51.09      75.00     0.083725
  19   51.35     200.00     0.095754   20   51.22      65.00     0.102590
  21   53.32      67.50     0.107979   22   49.35      67.50     0.104319
  23   48.01     200.00     0.106719   24   51.01      65.00     0.116018
  25   53.33      90.00     0.089596   26   53.22      70.23     0.092887
  27   54.17      67.50     0.117974   28   50.24      67.50     0.117709
  29   52.23      72.50     0.090946   30   50.08     122.50     0.108557
  31   48.44      81.25     0.117919   32   49.82      70.00     0.089918
  33   48.49     200.00     0.103319   34   50.55      85.00     0.099533
```

35	52.42	67.50	0.102156	36	50.34	72.50	0.090494
37	55.13	73.75	0.119052	38	53.85	77.50	0.090540
39	54.80	80.00	0.116289	40	50.01	71.67	0.088077
41	48.14	87.50	0.092156	42	46.12	66.88	0.082146
43	51.85	67.50	0.105659	44	50.47	71.67	0.076525
45	51.20	71.25	0.082111	46	47.23	100.00	0.108847
47	49.46	67.50	0.118949	48	52.38	67.50	0.080578
49	51.72	100.00	0.110247	50	47.38	200.00	0.083820
51	51.69	67.50	0.112709	52	54.84	82.50	0.112589
53	54.25	92.50	0.099372	54	53.91	75.83	0.109865
55	52.11	72.50	0.094126	56	47.26	92.50	0.084810
57	50.92	200.00	0.081427	58	48.58	200.00	0.107239
59	50.06	70.47	0.106571	60	47.75	76.25	0.093347
61	51.30	82.50	0.090452	62	48.86	67.50	0.069759
63	47.80	75.00	0.100669	64	48.13	97.50	0.092177
65	50.47	76.25	0.087248	66	48.30	87.50	0.103065
67	53.12	75.00	0.093665	68	49.60	90.00	0.083605
69	48.13	97.50	0.106620	70	51.19	74.38	0.085386
71	52.44	71.25	0.110362	72	54.32	70.00	0.100955
73	47.40	76.25	0.077629	74	54.49	83.75	0.104798
75	46.18	90.00	0.117672	76	53.76	135.00	0.118670
77	50.64	200.00	0.098460	78	52.42	70.00	0.104361
79	55.20	176.25	0.120645	80	52.01	73.33	0.106806
81	47.14	92.50	0.108908	82	49.87	67.50	0.096319
83	54.18	83.75	0.097787	84	53.90	67.50	0.112675
85	54.73	76.00	0.110134	86	46.94	83.75	0.113641
87	51.32	85.00	0.078882	88	53.07	200.00	0.113146
89	49.84	85.00	0.092655	90	51.30	81.25	0.109996
91	51.34	200.00	0.109759	92	49.94	77.50	0.093821
93	46.37	80.00	0.116513	94	53.40	200.00	0.099291
95	53.65	200.00	0.085961	96	52.61	70.00	0.119431
97	53.48	200.00	0.095086	98	47.87	72.50	0.088464
99	51.92	72.50	0.084792	100	51.75	70.00	0.095629
101	47.62	70.00	0.067451	102	44.90	112.50	0.109552
103	54.13	137.50	0.106843	104	50.54	80.00	0.119330
105	47.37	82.50	0.119126	106	52.50	200.00	0.114915
107	50.56	200.00	0.118188	108	45.82	92.50	0.102816
109	49.16	70.56	0.095406	110	54.98	82.50	0.115657
111	46.36	100.00	0.113325	112	54.16	95.00	0.097460
113	44.69	78.75	0.114221	114	51.59	95.00	0.078878
115	48.94	90.00	0.095149	116	53.07	200.00	0.103140
117	45.98	128.75	0.087437	118	54.43	105.00	0.103526
119	55.15	200.00	0.119653	120	48.88	71.75	0.086859
121	52.99	76.25	0.096147	122	50.47	71.43	0.098369
123	51.21	65.00	0.070645	124	47.95	66.88	0.072297
125	47.77	143.00	0.113119	126	53.49	76.25	0.101501
127	52.07	76.25	0.097811	128	52.42	67.50	0.068878
129	54.92	73.00	0.114331	130	48.86	200.00	0.106219
131	52.92	90.00	0.087813	132	52.82	70.77	0.098085
133	54.70	78.75	0.109444	134	52.74	67.50	0.073428
135	51.83	67.50	0.093177	136	48.87	91.88	0.088334
137	54.20	78.12	0.098379	138	51.81	97.50	0.083504
139	53.28	70.00	0.084294	140	51.59	67.50	0.057118
141	49.90	68.75	0.112481	142	47.35	132.50	0.111781
143	52.69	70.00	0.090320	144	49.72	71.67	0.076081
145	51.78	70.00	0.066182	146	54.26	93.33	0.099712
147	51.65	200.00	0.117938	148	45.10	78.33	0.106896
149	49.36	72.50	0.087871	150	46.43	72.50	0.105173
151	52.36	67.50	0.093487	152	52.83	88.75	0.106339
153	51.32	96.25	0.107205	154	51.39	107.50	0.101175
155	49.22	70.28	0.108470	156	52.72	72.50	0.107166
157	49.14	92.50	0.087067	158	54.67	76.25	0.108804
159	52.07	71.25	0.103306	160	50.89	82.50	0.107607
161	50.71	65.00	0.074855	162	49.49	90.00	0.110313
163	53.05	90.00	0.106991	164	48.53	69.00	0.077669
165	54.01	142.50	0.105233	166	51.87	67.50	0.075038

```
167   51.42     72.00     0.086779  168  51.23     87.50     0.091750
169   53.52    200.00     0.110353  170  50.40     67.50     0.083134
171   47.76     75.00     0.116332  172  52.04     67.50     0.096646
173   49.96     95.00     0.105776  174  52.55     78.75     0.106479
175   47.15    102.50     0.085287  176  54.61     70.00     0.118001
177   55.00     78.75     0.116102  178  49.54     86.25     0.082003
179   53.15    110.00     0.104589  180  51.47     72.50     0.092080
181   53.79     95.00     0.094254  182  52.77     85.00     0.090763
183   51.93     70.00     0.079519  184  45.86     67.50     0.091969
185   48.60    200.00     0.116270  186  49.75     78.33     0.093030
187   48.84     67.50     0.099911  188  54.29    120.00     0.106461
189   48.49    101.25     0.106505  190  51.70     67.50     0.103941
191   53.31     67.50     0.111284  192  54.48     71.88     0.104502
193   53.05     70.00     0.072732  194  54.93     76.67     0.114565
195   54.83     71.25     0.112500  196  53.68    127.50     0.099501
197   52.34     76.25     0.078869  198  51.28     67.50     0.110979
199   47.65     70.00     0.120002  200  52.51     85.00     0.113096
201   54.74    200.00     0.113200  202  51.60     67.50     0.096155
203   50.24     90.00     0.095530  204  53.49     67.50     0.111722
205   44.41    137.50     0.120483  206  54.09    200.00     0.095969
207   53.57     85.00     0.114420  208  47.37     76.25     0.092365
209   49.27     70.00     0.106445  210  48.16     70.62     0.111745
211   49.81    105.00     0.112147  212  49.53     70.00     0.075259
213   53.05     93.75     0.072566  214  46.59    200.00     0.108372
215   51.84    101.25     0.091232  216  54.59    200.00     0.107136
217   53.62     67.50     0.085424  218  51.86     70.00     0.073674
219   48.96     67.50     0.118105  220  50.45     65.00     0.076182
221   50.89     71.25     0.104087  222  54.36     75.83     0.101823
223   53.18    200.00     0.101965  224  51.02    200.00     0.095974
225   49.82    200.00     0.083916  226  54.13     75.00     0.119927
227   53.86     74.77     0.098235  228  48.16     70.00     0.078794
229   51.50     67.50     0.071126  230  54.05     82.50     0.098923
231   54.54    108.75     0.105969  232  49.18     97.50     0.117451
233   53.40     67.50     0.099686  234  53.98     67.50     0.111116
235   54.21     67.50     0.098638  236  53.92     80.00     0.092133
237   52.81    117.50     0.107397  238  54.68     73.75     0.109118
239   53.85     87.50     0.113659  240  52.94     67.50     0.081391
241   52.71     67.50     0.092480  242  53.11     75.00     0.088589
243   52.59     78.75     0.101356  244  49.37     71.67     0.115067
245   55.06    200.00     0.117549  246  53.99     70.00     0.093629
247   50.68     67.50     0.093188  248  55.02     80.00     0.116731
249   44.84     77.50     0.110893  250  46.09     98.75     0.108497


EXPONENTIAL MEAN TEMPERATURE SOLUTION:
OBSERVED AFT AGE =  49.8 MA  CALCULATED AFT AGE =  51.1 MA
MODEL CLOSURE AGE =  72.5 MA  OBJ FUNCTION =      0.120645


MINIMUM OBJECTIVE SOLUTION:
CALCULATED AFT AGE =  51.6 MA  MODEL CLOSURE AGE =  67.5 MA
OBJ FUNCTION =      0.057118


CLOSURE AGE DISTRIBUTION FOR ALL ACCEPTABLE SOLUTIONS:
AVE AFT AGE =  51.2 MA
AVE MODEL CLOSURE AGE =  95.4 +/-  41.7 MA

    AGE BIN       RELATIVE
     (MA)        FREQUENCY
  50.0 -  55.0     0.000
  55.0 -  60.0     0.000
  60.0 -  65.0     0.024
  65.0 -  70.0     0.244
  70.0 -  75.0     0.180
  75.0 -  80.0     0.116
```

80.0 - 85.0	0.072
85.0 - 90.0	0.064
90.0 - 95.0	0.036
95.0 - 100.0	0.040
100.0 - 105.0	0.024
105.0 - 110.0	0.020
110.0 - 115.0	0.012
115.0 - 120.0	0.008
120.0 - 125.0	0.004
125.0 - 130.0	0.008
130.0 - 135.0	0.008
135.0 - 140.0	0.008
140.0 - 145.0	0.008
145.0 - 150.0	0.000
150.0 - 155.0	0.000
155.0 - 160.0	0.000
160.0 - 165.0	0.000
165.0 - 170.0	0.000
170.0 - 175.0	0.004
175.0 - 180.0	0.004
180.0 - 185.0	0.000
185.0 - 190.0	0.000
190.0 - 195.0	0.000
195.0 - 200.0	0.000

OBSERVED TRACK LENGTH HISTOGRAM:

BIN SIZE (MICRONS)	RELATIVE FREQUENCY
0.0 - 1.0	0.000
1.0 - 2.0	0.000
2.0 - 3.0	0.000
3.0 - 4.0	0.000
4.0 - 5.0	0.000
5.0 - 6.0	0.000
6.0 - 7.0	0.000
7.0 - 8.0	0.008
8.0 - 9.0	0.000
9.0 - 10.0	0.024
10.0 - 11.0	0.165
11.0 - 12.0	0.260
12.0 - 13.0	0.323
13.0 - 14.0	0.181
14.0 - 15.0	0.039
15.0 - 16.0	0.000
16.0 - 17.0	0.000
17.0 - 18.0	0.000
18.0 - 19.0	0.000
19.0 - 20.0	0.000

APPENDIX IV - PLOTS

This sections contains example plots showing results for a model run using the Amerk O-09 data. The six plots generated during execution of the batch routine, GOFTPLT, are AVET (p. 71), ALLT (p. 72), MINT (p. 73), PDF (p. 74), ALLPDF (p. 75) and CLOS (p. 76). These plots are produced as screen versions (by execution of ZPVIEW), as Postscript output (using ZPPOST) and as DXF format files (using ZPLOT). Figures IV.1-IV.6 are the DXF versions which were imported into CORELDRAW, exported as Wordperfect format files (WPG) and imported into this document.

Figure IV.1 shows a plot of the exponential mean (preferred) thermal solution plus the bounding temperature envelopes containing all statistically acceptable solutions. The pronounced decrease in temperature at 40 Ma results from the requirement that the sample had to be at surface temperatures during deposition. Prior to deposition, the thermal history is poorly constrained. The model indicates rapid heating to the present maximum temperature during the last 2.5 m.y. model time step (~11 °C/m.y.), a feature shown by all models (Fig. IV.2). Figure IV.2 shows all 250 solutions that were used to define the acceptable solution space. Note that these results depend on the chosen model parameters. If more time steps were added and calculated maximum rates were used, the acceptable solution space would increase with more widely flucuating thermal solutions. However, it is an open question whether this would provide a more geologically meaningful result.

The minimum objective solution is shown in Figure IV.3 (see Appendix III for a discussion of this solution). Figure IV.4 shows the probability density function (calculated track length distribution) for the preferred thermal history superimposed on a histogram of measured track lengths. Note that the actual fit to the data is based on the cumulative density function (sum of ordered tracks) using the Kolmogorov-Smirnov statistic. The bounding envelope of track length distributions shown in Figure IV.4 was derived from the acceptable family of length distributions (Fig. IV.5). Figure IV.6 shows a plot of model closure ages for all acceptable solutions in Figure IV.2 (see Appendix III for a brief discussion of closure ages).

Figure IV.1 - AVET

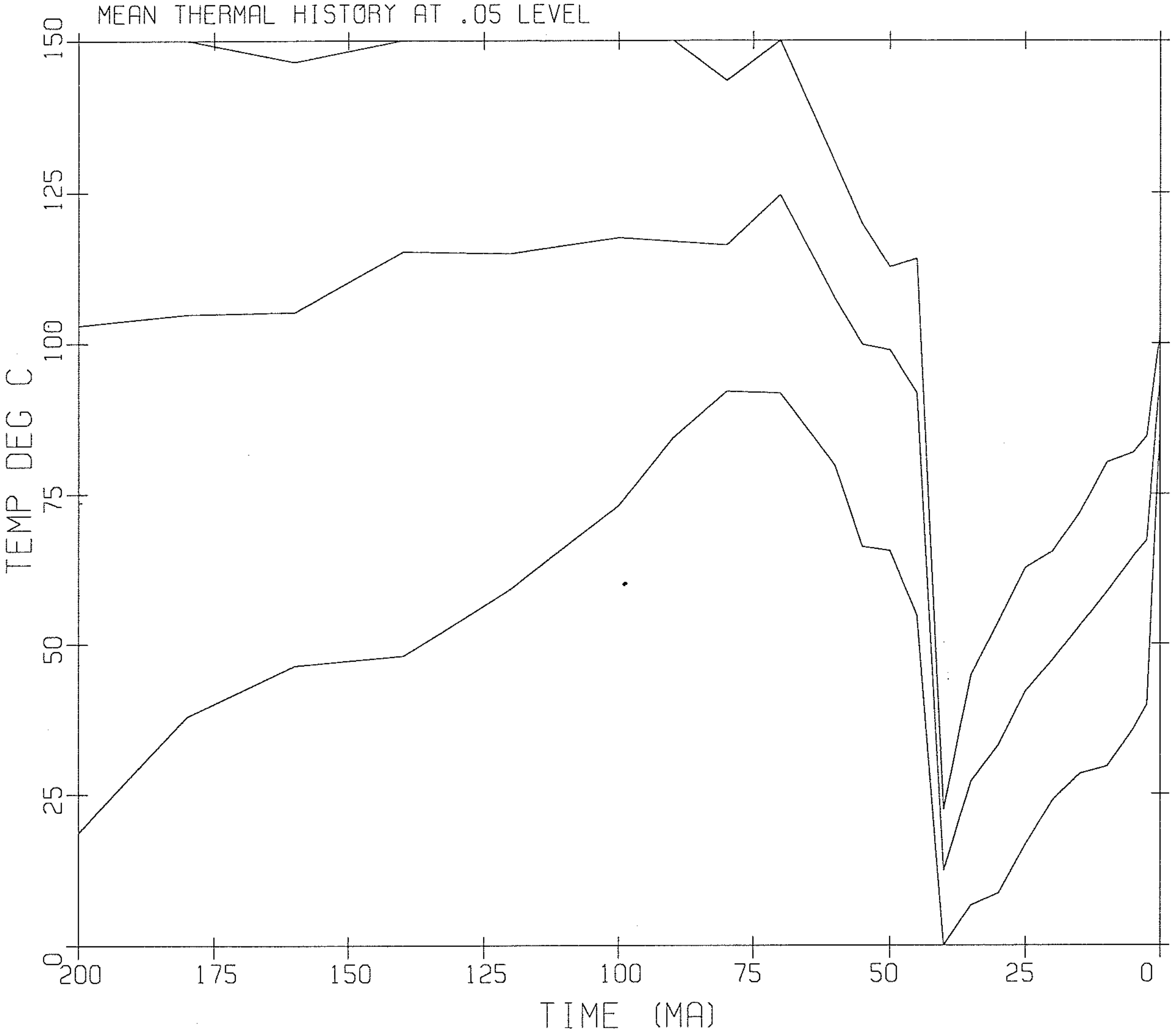


FIGURE IV.2 - ALLT

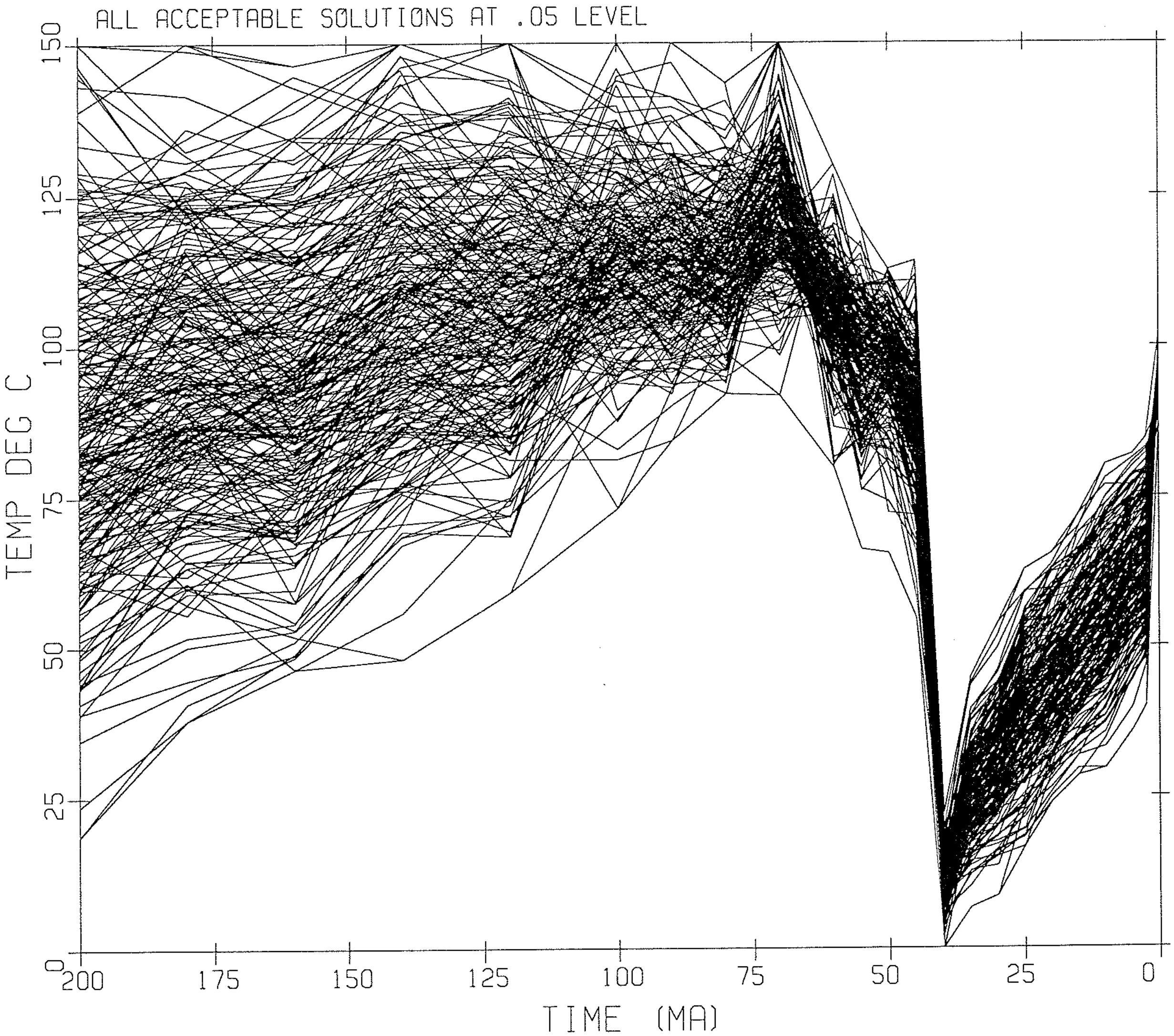


FIGURE IV.3 - MINT

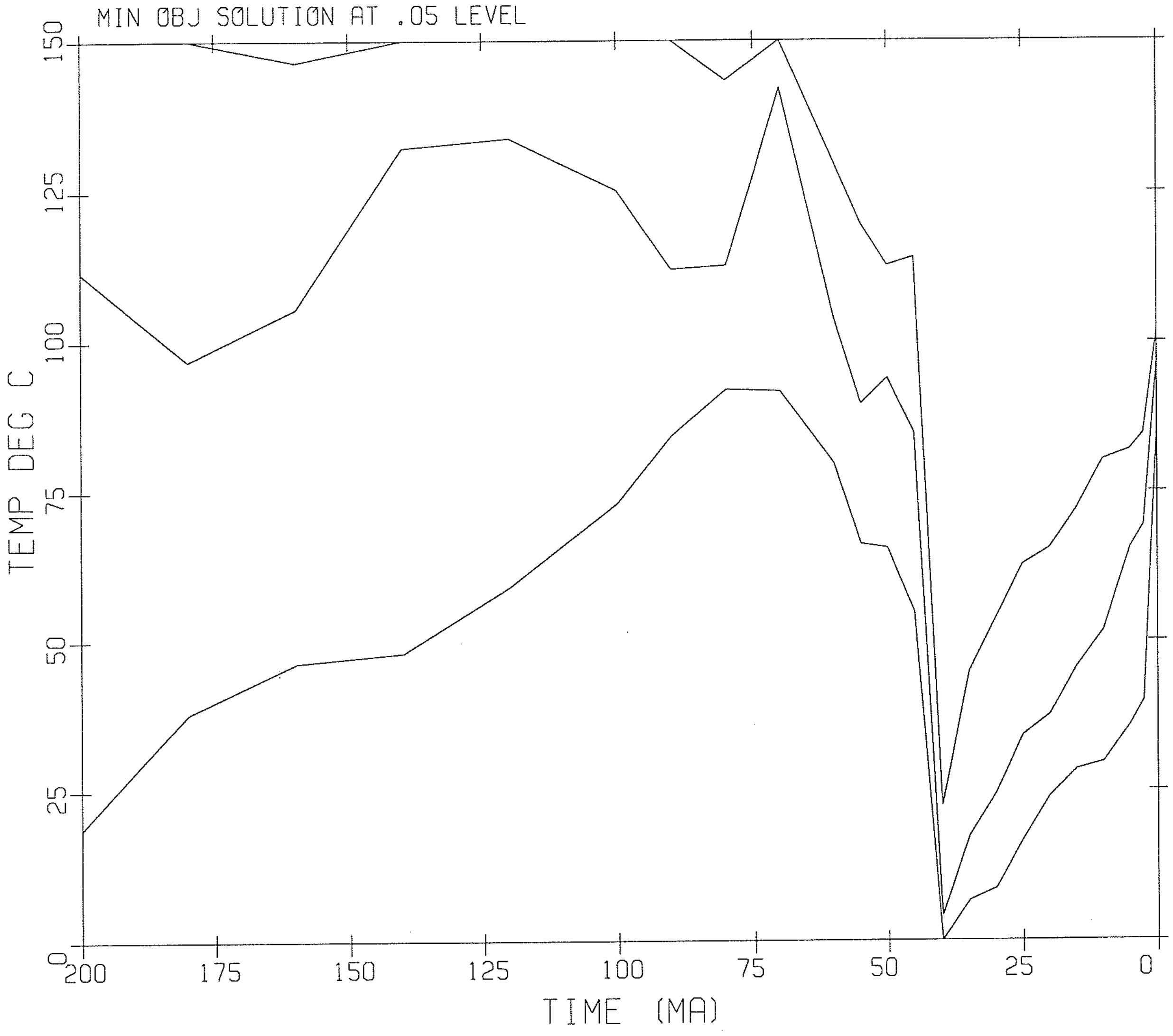


FIGURE IV.4 - PDF

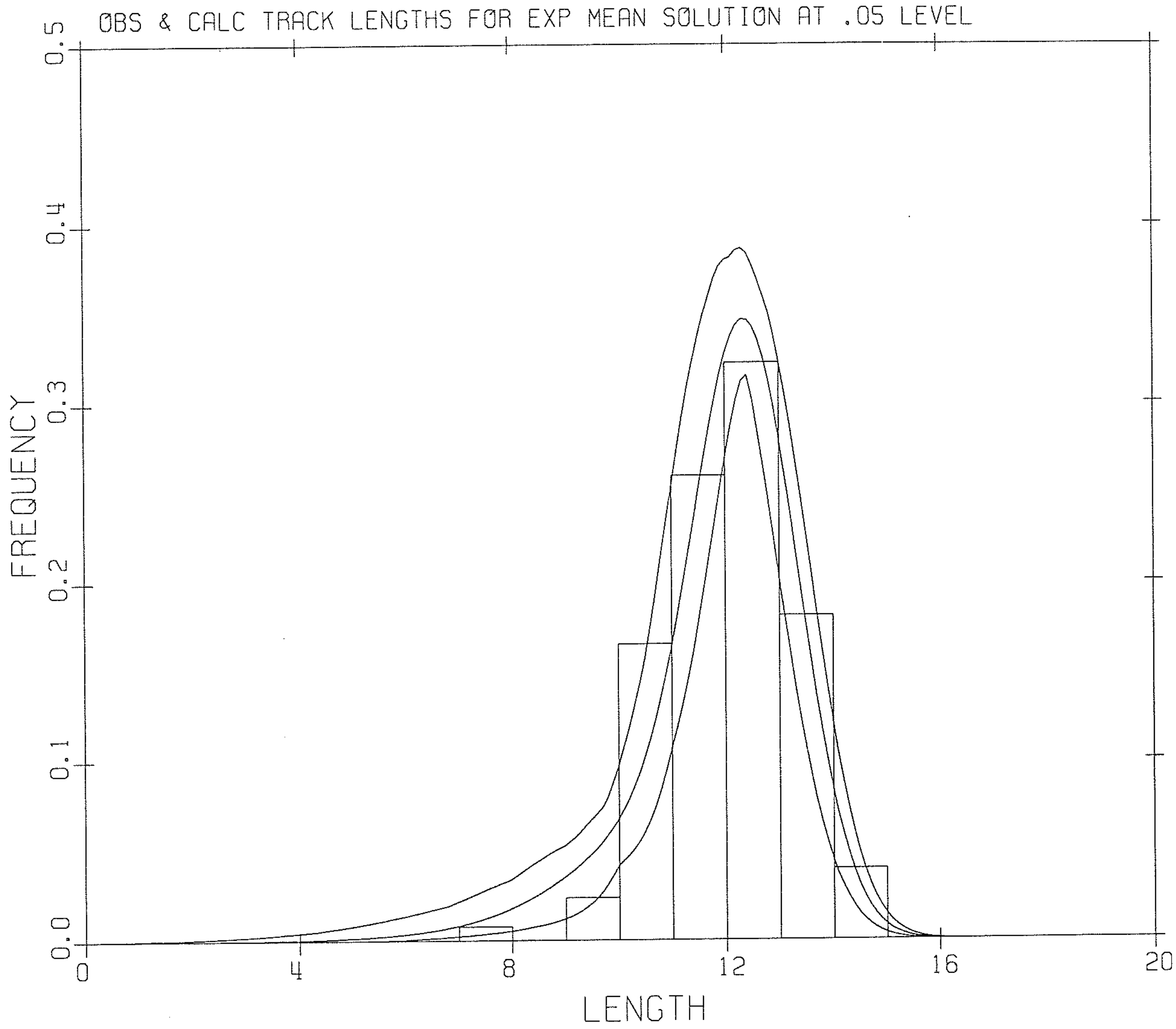


FIGURE IV.5 - ALLPDF

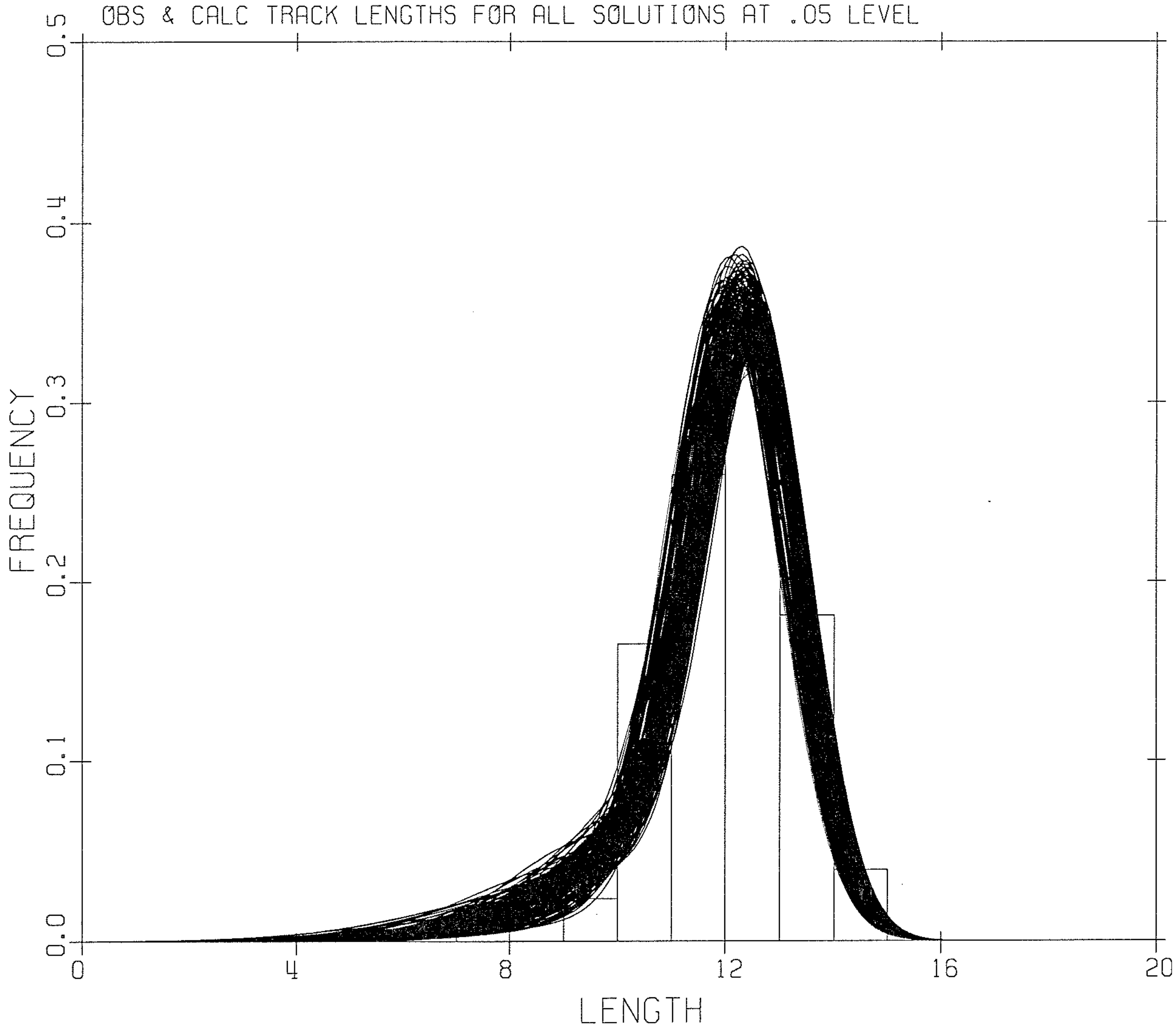
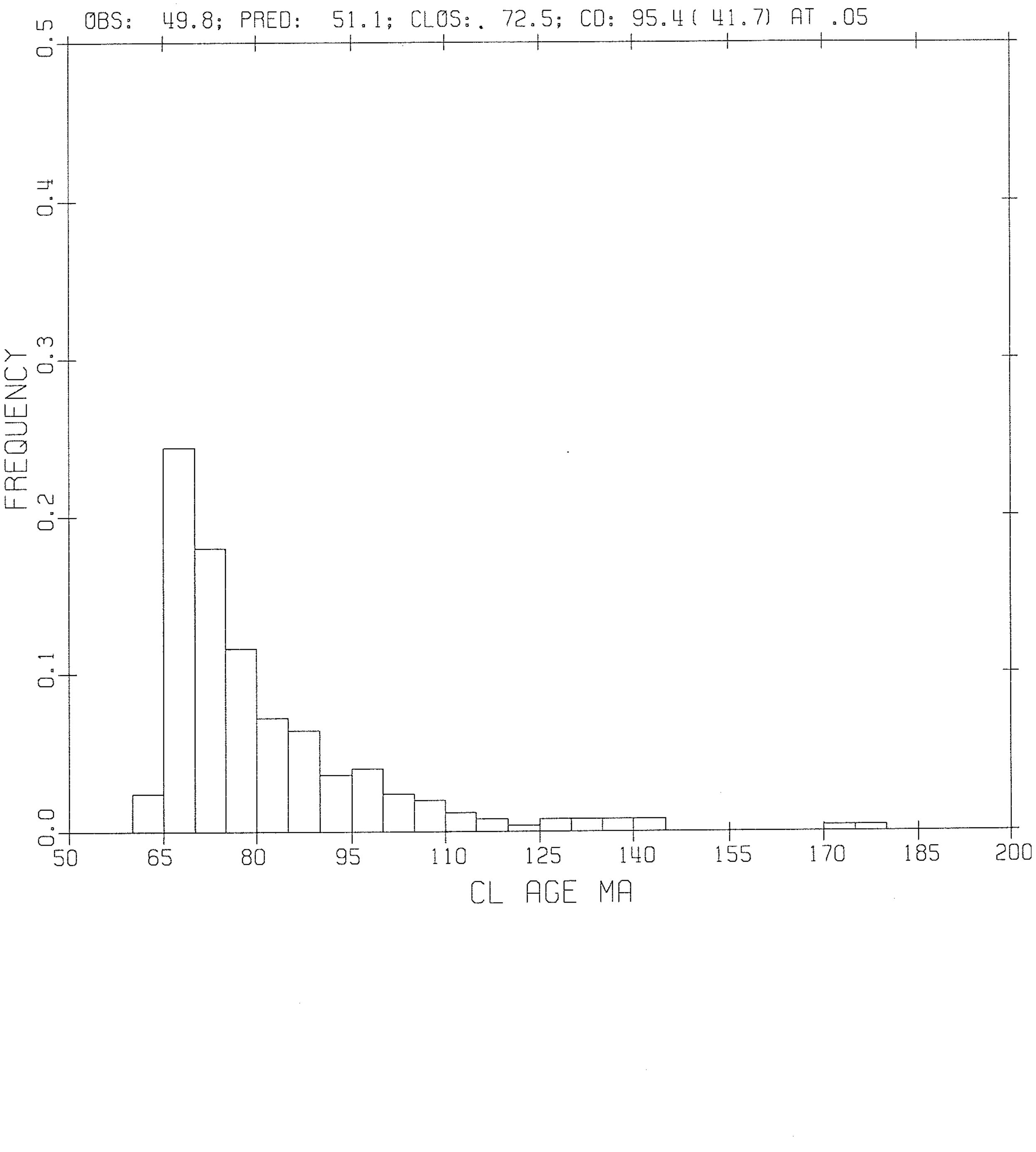


FIGURE IV.6 - CLOS



APPENDIX V - TIME STEP PREDICTOR FUNCTION

The 6-parameter annealing equation of Crowley *et al.* (1991),

$$\frac{[(1-r^{\beta})/\beta]^{\alpha} - 1}{\alpha} = C_0 + \frac{C_1 \ln(t) + C_2}{1/T - C_3} \tag{V.1}$$

is used in the inverse model, AFTINV32, to calculate apatite fission track annealing as a function of temperature. For Equation V.1, r is the normalized reduced track length (final/initial track length), T is temperature (K), t is time (s), and α, β, C_0, C_1, C_2 and C_3 are parameters corresponding to specific apatite compositions. The isothermal annealing model (Equation V.1) can be solved for variable thermal histories using the method of equivalent time (Goswami *et al.*, 1984; Duddy *et al.*, 1988). In this solution technique, track annealing is assumed to depend on the current state of annealing and the prevailing time-temperature conditions only, and is independent of the previous time-temperature path which led to its present state of annealing.

The amount of fission track annealing can be calculated by appropriate rearrangement of Equation V.1 and by approximating a given thermal history as a series of isothermal steps. The solution method is based on using the amount of annealing, as determined in a previous step, to calculate the equivalent time spent at the temperature for the current step and this process is repeated for the entire thermal history. A time step predictor function (Issler, 1996),

$$S = \frac{\left(\sqrt{\ln(T_a/T_m)/A_1} + A_2 e^{-(T_m - T_a)/A_3}\right)}{R^{A_4}} \tag{V.2}$$

is used to discretize the thermal history into isothermal steps for efficient and accurate evaluation of Equation V.1. In Equation V.2, S is the isothermal time step size (m.y.) as a function of maximum interval temperature (T_m in K), total annealing temperature (T_a in K) and rate of temperature change (R in K/m.y.). Coefficients A_1 to A_4 are determined individually for apatites with different compositions and annealing characteristics. The total annealing temperature, T_a, is defined as the temperature at which tracks are reduced to effectively zero length and is given by,

$$T_a = A_5 R^{A_6} \tag{V.3}$$

where constants A_5 and A_6 must be determined for apatites having a specific composition and associated annealing behaviour.

It should be noted from Equation V.3 that T_a decreases with decreasing rate of temperature change and that for very low values of R (near isothermal condition), T_a can be a small number. When T_m is greater than or equal to T_a, Equation V.2 is no longer valid. However, before one can assume complete track annealing, it is necessary to compare the duration of the model time interval with the time required to isothermally anneal a track at temperature T_a. If the theoretical isothermal annealing time is less than or equal to the model time, tracks are assumed to be completely annealed. In contrast, if the isothermal annealing time is much greater than the model time (as may be the case for very slow temperature changes), then Equation V.2 is evaluated at a temperature, T_a -0.01 K, and the resulting value of S is used to discretize the model time interval.

Coefficients A_1 to A_6 in equations V.2 and V.3 were determined according to the procedures described in Issler (1996). Numerical data were generated for different annealing models at constant heating rates over selected temperature ranges such that calculated values of r were within 0.1% of the "true" r value. From these data, T_a values were determined for different heating rates and were fit to a power function relating T_a and

R (Equation V.2). A nonlinear optimization technique (Levenberg-Marquardt method; see Press *et al.*, 1986) was used to determine coefficients A_1 to A_4 for Equation V.2. Table V.1 lists the values of coefficients A_1 to A_6 that were determined for the (1) Durango, (2) Sr fluorapatite and (3) fluorapatite annealing models of Crowley *et al.* (1991) and the (4) Durango model of Laslett *et al.* (1987). Figure V.1 shows the relation between T_a and heating rate for models 2, 3 and 4. Figures V.2, V.3 and V.4 show the results of fitting numerically generated S data (at 0.1% accuracy level) with Equation V.2 for models 2, 3 and 4 above, respectively (results for model 1 are shown in Figure 2 in the section, Programs). Overall, these results indicate that resistance to annealing increases in the following order: Durango (Laslett *et al.*, 1987); Durango (Crowley *et al.* 1991); fluorapatite (Crowley *et al.*, 1991) and Sr fluorapatite (Crowley *et al.*, 1991).

The coefficients in Table V.1 are given for the 0.1% accuracy level (with respect to the true value of r) but can be scaled to other accuracy levels by multiplying S values by the factor $(10E)^{1/2}$, where E is the approximate accuracy for calculated r values. Although users are allowed to input their own annealing model coefficients (C_1,C_2,C_3,C_4,α,β), they must also change the corresponding time step function coefficients (A_1 to A_6) which are used to evaluate the selected annealing model. Otherwise, model calculations may be inaccurate. At a minimum, changes to coefficients A_5 and A_6 are necessary to reflect the new relationship between T_a and R because these parameters have the most influence on calculated differences in S values among different annealing models.

Table V.1 - Time step function coefficients.

Step Size Coefficients	Annealing Model			
	Laslett et al. (1987)	Crowley et al. (1991)		
	Durango	Durango	Fluorapatite	Sr Fluorapatite
A_1	0.00687	0.00596	0.00435	0.00407
A_2	0.117	0.043	-0.00497	-0.0845
A_3	38.7	34.8	67.0	83.9
A_4	0.981	0.978	0.977	0.977
A_5	393.18	398.15	412.34	428.91
A_6	0.0162	0.0157	0.0135	0.0128

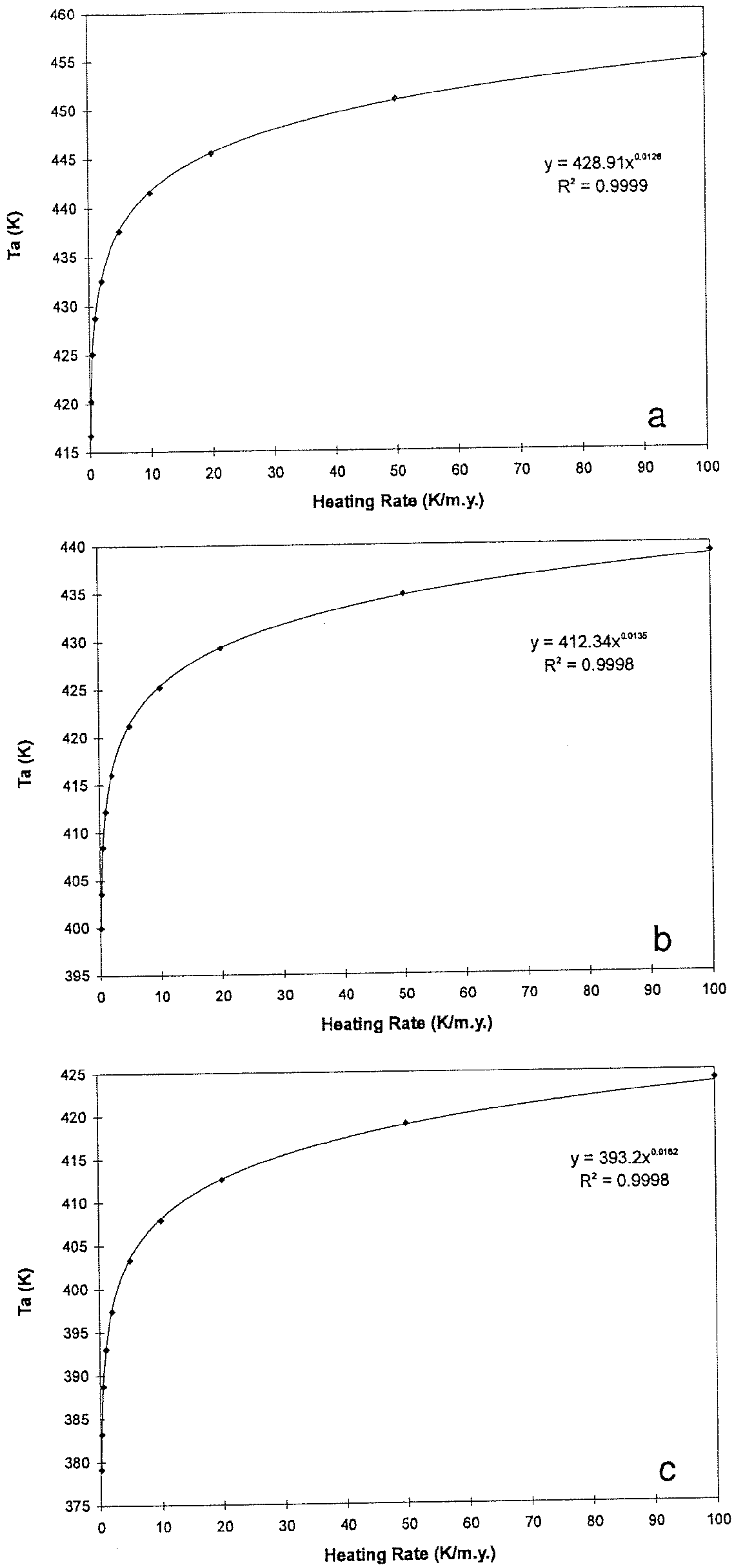


Figure V.1. Total annealing temperature versus heating rate for a) Sr fluorapatite (Crowley *et al.*, 1991), b) fluorapatite (Crowley *et al.*, 1991) and c) Durango apatite (Laslett *et al.*, 1987).

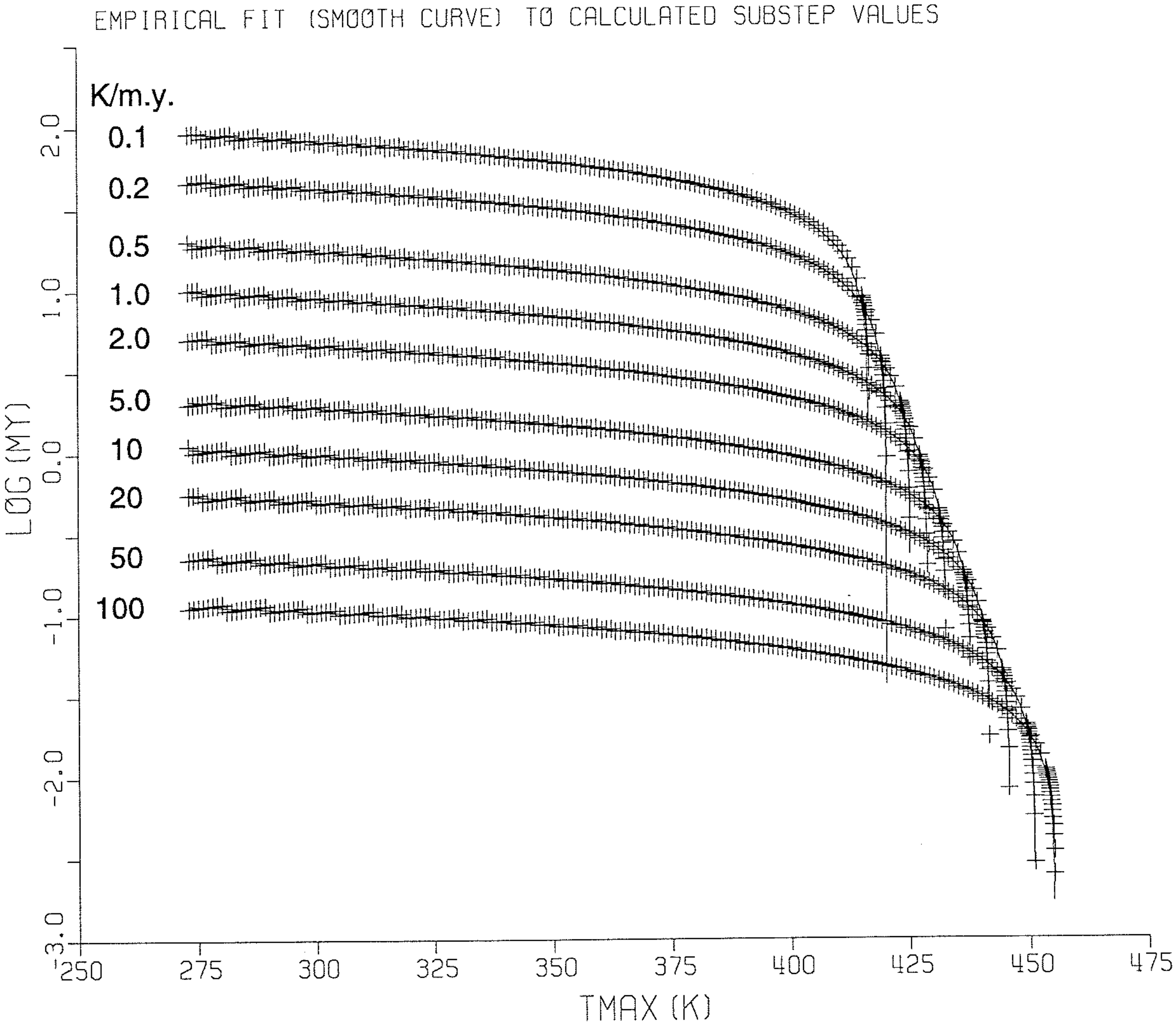


Figure V.2. Logarithm of isothermal time step size (S) versus maximum interval temperature for selected heating rates ranging from 0.1 to 100 K/m.y. for the Sr fluorapatite annealing model of Crowley et al. (1991). Numerical data (crosses) are for the 0.1 % accuracy level and calculated values (solid curves) are from equation V.2 using the parameters in Table V.1.

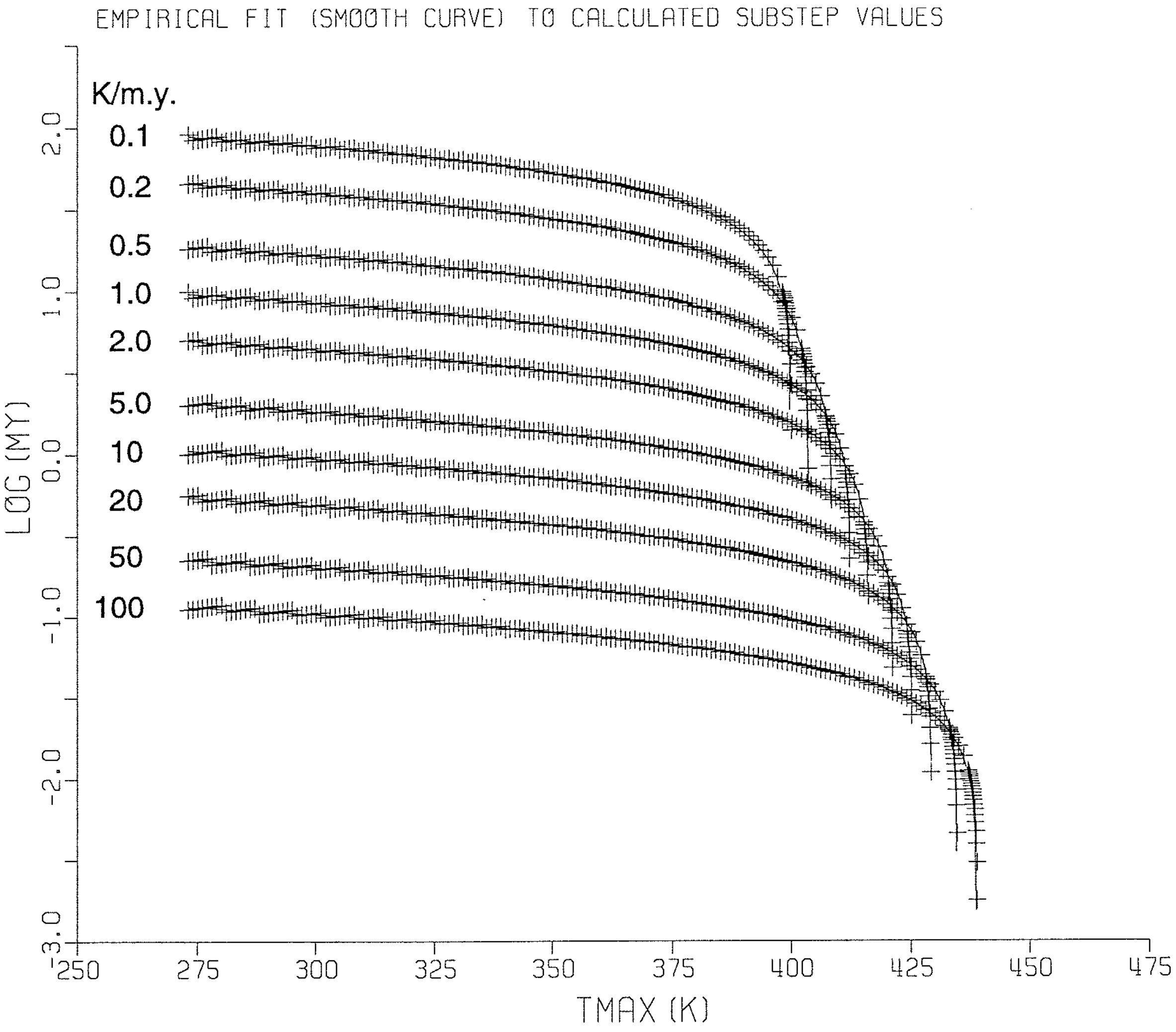


Figure V.3. Logarithm of isothermal time step size (S) versus maximum interval temperature for selected heating rates ranging from 0.1 to 100 K/m.y. for the fluorapatite annealing model of Crowley et al. (1991). Numerical data (crosses) are for the 0.1 % accuracy level and calculated values (solid curves) are from Equation V.2 using the parameters in Table V.1.

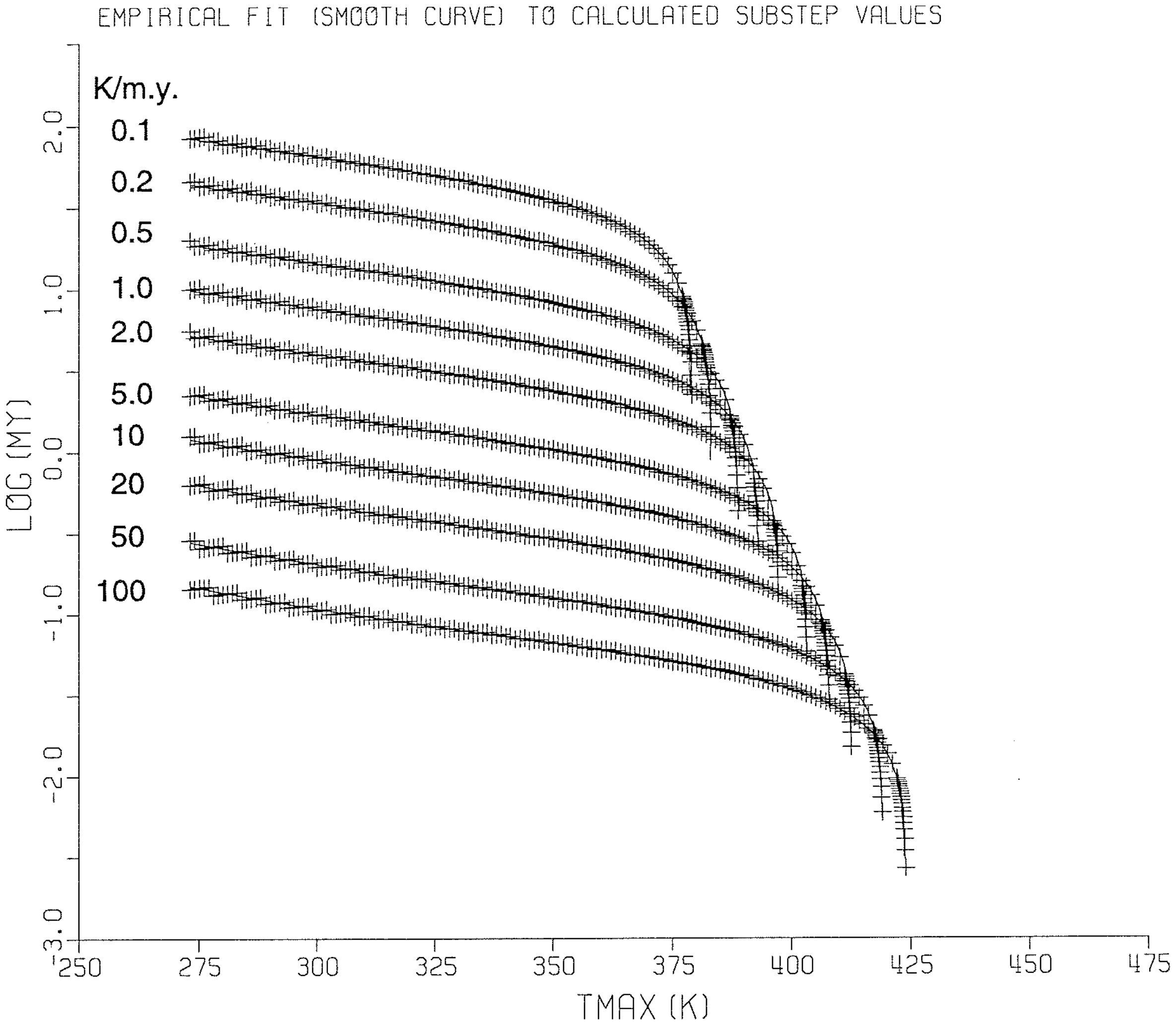


Figure V.4. Logarithm of isothermal time step size (S) versus maximum interval temperature for selected heating rates ranging from 0.1 to 100 K/m.y. for the Durango annealing model of Laslett et al. (1987). Numerical data (crosses) are for the 0.1 % accuracy level and calculated values (solid curves) are from equation V.2 using the parameters in Table V.1.