4DTHERM

Version 1.2

— Inverse Thermal Modeling of Geo-/Thermochronology Data

Users Manual

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1. Introduction

4DTHERM ***1.2*** is an inverse thermal modelling software package developed by Frank Q. Fu as part of his PhD study at the University of Sydney in cooperation with Brent McInnes and Noreen Evans of CSIRO Australia. It is a 2D explicit finite difference solution which addresses conduction cooling, latent heat of crystallization/fusion, thermal convection within magma bodies, and hydrothermal circulation induced by magma intrusion as well as exhumation and erosion processes.

Main Applications

The primary application of this program is to derive thermal and exhumation histories of igneous intrusions directly from multiple geo-/thermochronometers by utilizing numerical modeling techniques. The outputs will quantify a number of parameters related to the dynamic processes of magmatic-hydrothermal cooling, the timing and duration of hydrothermal activity, and the denudation history of igneous intrusions and related mineralization (Fu et al., 2005; McInnes et al., this volume; McInnes et al., 2005).

4DTHERM ***1.2*** can simulate the conductive and convective cooling processes of igneous bodies. It computes the distributions and variations of temperature in both igneous bodies and country rocks throughout the whole cooling process. It records the time and duration of magmatic-hydrothermal activity induced by intrusions. It also records the cooling history and calculates the cooling rate for some pre-defined positions (e.g. sample and tracer positions in igneous bodies and/or country rocks).

Main Features

- **Platform Independent**

  4DTHERM ***1.2*** was implemented in Java programming language and is, thus, platform-independent. It has been tested in Windows ME, XP, Linux/Unix OS and Mac OS X, and should be able to run on other operating systems.

- **Well-Designed GUI**

  It has a well-designed, interactive graphical user interface (GUI) for observing modeling processes and controlling modeling procedures. The appearance and layout of the GUI can be changed at any time. Popup menus containing a set of shortcuts can be opened by right-clicking on the windows and the time scales can be changed by mouse-dragging. Most buttons and check boxes will display tool tips while the mouse is positioned over them and are self-explanatory.

- **Powerful Auxiliary Tools for Data Input and Output**

  It provides a set of auxiliary facilities for constructing geologic units, inputting and modifying computational parameters, editing model scenarios, and defining monitoring devices (tracers). It also provides a "Cooling Curve Viewer" tool to view, analyse and compare the final modeling results.

- **Dynamic Modeling and Visualization**

  Modeling processes can be run in automation mode and instant modeling results can be visualized at each time step.

- **Utilizing Geo-/Thermochronology Data**

4DTHERM *1.2* utilizes high-precision geo-/thermochronometry data to constrain inverse modeling of the thermal history of an igneous intrusion or magmatic-hydrothermal ore deposit. These age data are also used to calculate the exhumation and erosion rates and to reveal the intrusion's exhumation history.

- **Modeling Combined Cooling Processes**

4DTHERM *1.2* simulates the conductive and convective cooling processes of igneous bodies. It can address conductive cooling, thermal convection within a magma of limited volume, hydrothermal circulation in porous media, the release of latent heat, exhumation and erosion cooling, etc.

2. Setup of 4DTHERM *1.2*

2.1. System Requirements

4DTHERM *1.2* was implemented in Java language, is platform-independent and can be run on most operating systems. The recommended minimum and desired hardware configurations are:

Hardware	Minimum	Desired
RAM	128 MB	256 MB
Hard Disk	1 GB	5 GB
Screen Resolution	1024×768 pixels	1400×1050 pixels
Color	16 bit	32 bit

2.2. Supporting Software

4DTHERM *1.2* has not yet been packaged as an executable application. It has to be run by inputting command lines in a terminal window (a program running command lines, also called command prompt). To run **4DTHERM**, your machine needs a terminal window and should support the Java runtime environment (JRE, version 1.4 or higher). Fortunately, most Linux/Unix machines have built-in terminal windows and support Java runtime environment. Microsoft Windows ME/XP machines have MS-DOS prompt windows which can be used to input command lines.

Install a Terminal Window

If your machine does not have a terminal window installed, then you need to install one. For Windows OS, it is recommended to install Cygwin which is a Windows-based Linux/Unix terminal window and easy to use.

Cygwin is free software and you can download/install it from http://cygwin.com/ by simply clicking the "download" link on this page and then following the instructions.

Install Java

If your machine does not have Java installed already, you need to download version 1.4 or higher of Java from http://java.sun.com/j2se/1.4/download.html (also free software). Both Java SDK and JRE are available from this website. The Java SDK (Software Developers Kit) is used to compile and to run Java programs and the JRE (Java Runtime Environment) is used only for running Java programs that have already been compiled.

4DTHERM *1.2* provides compiled Java classes so you can download either the JRE or the SDK. Choose the download that is most suitable for your operating system, and then follow the instructions to install Java.

To check whether Java has been installed properly, open a terminal window, type “java Hello” and press “Enter” key. If the text displayed in the terminal window is something like “Exception in thread "main" java.lang.NoClassDefFoundError: Hello”, then the installation of Java SDK is successful. If the text displayed is something like “bash: java: command not found”, you may need to set the path in the system.

2.3. Setup Instructions

Unzip/extract the “4dtherm1.2.zip” archive into the directory of your choice. Files and directories extracted from “4dtherm1.2.zip” are all in a directory named “4dtherm1.2” which contains a subdirectory named “uni”, a Users Manual, a Readme text file, a Makefile file and a subdirectory named “examples”. The “uni” subdirectory contains all compiled java classes. The “examples” subdirectory contains example input/output files. You may move or rename the “4dtherm1.2” directory at any time if desired. However, for your convenience, it is recommended that the “4dtherm1.2” directory be in the same directory as the terminal window’s working directory. This will save you time when running the software.

To find out the working directory of a terminal window, input “pwd” after having opened a terminal window. The working directory will then be printed in the window. For example, input “pwd” and press the “Enter” key in a Cygwin window, the text *“/cygdrive/c/Documents and Settings/users*” will be printed in the window, which indicates that the main working directory of Cygwin program is “users”. So, the “4dtherm1.2” should be a subdirectory of the directory “users”.

3. Getting Started

3.1. Quick Start 4DTHERM *1.2*

After having installed Java, and downloaded and unzipped “4dtherm1.2.zip”, you are now ready to start **4DTHERM**. Starting **4DTHERM** is very simple and straightforward:

a) **Open a terminal window, e.g., Cygwin window**

b) **Input command “cd 4dtherm1.2” and then press “Enter” key**

   If the directory (or folder) “4dtherm1.2” is not under the current working directory, the message of “bash: cd: 4dtherm1.2: No such file or directory” will be displayed in the terminal window. In this case, you can use “cd ..” command to move up one level to the parent directory of the current directory or “cd *subdirectory*” to move down one level to a child directory under the current directory (“*subdirectory*” should be replaced by the actual name of the child directory that you want to move into), until the “4dtherm1.2” directory is the current working directory.

c) **Input command “make”, press “Enter” key**

   If you see the message “bash: make: command not found” in the window, it means that the terminal window you are using does not support the “make” command. Do not worry, you can still run the software by manually typing the long command line "java -mx128m uni/ModelDriver".

Wait a few seconds, and then you will see a graphic user interface (GUI) appearing on the screen. Up to here, everything is going well and **4DTHERM** is ready to run.

3.2. Run the Model

To open a Cooling/Exhumation model window, click the "Models" menu, and choose "Cooling/ Exhumation" submenu.

When running the "Cooling/Exhumation" model, the following steps should be followed in order:

a) **Configure model resolution and modify parameters**

Click the "Settings" menu button in the Toolbar, or choose "Options" > "Parameter Settings" from the Menu Bar to open a Parameter Settings Panel. Configure the model domain and resolutions, change or modify parameters in the panel. If any values have been changed, do not forget to press the "Apply" button on the bottom of this panel to enforce these changes.

b) **Load a data file that contains geo-/thermochronology data**

Click the "Load" button in the Toolbar, or choose "File" > "Load" from the Menu Bar. In the "Load Data From" dialog box, select a file that contains geo-/thermochronology data, and click Load. Once data has been successfully loaded from the selected file, you will see that the name of the intrusion and all age data points are drawn in the History Window, and all samples' legends are shown in the Legend Panel.

c) **Construct an igneous body (or bodies) and/or country rocks**

Click the "Builder" button in the Control Panel, and then construct country rock and igneous bodies through the Geobody Building Panel. Once a geobody has been constructed, you will see the body drawn in the Viewing Window. For details, see Section 5.6.1 "How to Build a Geobody".

d) **Define tracers to observe the changes in temperature at the defined positions**

Open a Tracer Defining Panel to define tracers, or use mouse to directly define a tracer in the Viewing Window. For details, see Section 5.6.2 "How to Define a Tracer".

e) **Run the model**

Press the "**>>**" button in the Control panel to run the cooling process. To run the process automatically, toggle on the "Automation" radio box and then press the "**>>**" button. To pause the process, press "**||**" button; to restart a modeling process and/or to clear the constructed igneous bodies, press "Reset" button.

The above steps should be operated in order except (a) and (b) which are interchangeable. Once an igneous body has been built up, you are not allowed to change any parameters or load any new age data. Once the model has started running (i.e. step > 0), you cannot define any new tracers, or move or delete any tracers that have been already defined. Be aware that due to the complexity of the calculations, it may take up to one hour or more to obtain a final result depending on the resolution of the model and the geological time length to be modeled.

4. Menus, Toolbar and Status Bar

4.1. Layout of **4DTHERM** *1.2*

4DTHERM *1.2* has a well-designed, user-friendly graphic user interface. It consists (from the top to the bottom of the interface) of a Menu Bar, a Toolbar, a main window, and a Status Bar. The Menu Bar, Toolbar and Status Bar are the common GUI components for all models and will be introduced in this section. The main window may contain one or more modeling windows, a Legend Panel (optional), a Control Panel (optional), and will be examined in the next section.

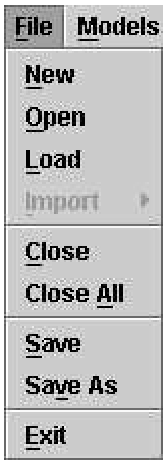
The layout of the GUI of 4DTHERM ***1.2***

4.2. Menu Bar

The Menu Bar is on the top of the interface. It consists of five menu groups and each group contains of a list of menu items that perform specific functions.

4.2.1. File Menu

This menu includes a list of items performing the basic I/O operations, including New, Open, Load, Import, Close, Close All, Save, Save As, and Exit.



New

Open a new (blank) text file for creating or editing input data file.

Open

Open an ASCII text file for viewing or editing. Click this button to open an "Open File" dialog box for selecting a file. The content of the selected file will be displayed in the text editor window after clicking the "Open" button in the dialog box.

Load

Load data (either raw data or resultant data) from a formatted ASCII text file into a model for processing.

Import

Import allows 3D models to read computed data (e.g. 3D graphic files/scenes) from some formatted files (e.g. VTK and obj files). Ignore it in this version of the software.

Close

Use this item to close the currently visualized modeling window. If the model is running at the moment when you click the “Close” menu item or button, a Confirm Dialog Box will pop out to ask you that “Cooling/Exhumation model is running. Do you want to end it now?”. If the model has already started running, a dialog box will pop up and ask “Modeling state has been modified. Do you want to save it?”. If you chose to save the results, they can be investigated at a later time. If you do not want to save the results, then go directly to set up the next test run.

Close All

This item closes all open modeling windows. However, when closing each individual modeling window, the program will confirm your intention by posing the same question it would if the model was running or had been modified (see above).

Save

Save the modeling results, including all initial settings, into a selected file.

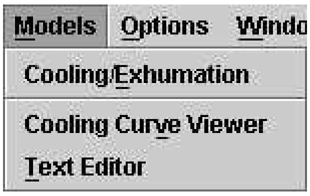
Save As

Save the current modeling results, including all initial settings, into a new file with specified file name. If the selected file name exists, previous data in this file will be overwritten by the new results to be saved.

Exit

Exit the software. It will first perform the “Close All” operation if there are opened modeling windows, and then pop out a Conform Dialog Box to ask you that “Do you want to exit **4DTHERM** now?” before exiting.

4.2.2. Models Menu



It includes three menu items: Cooling/Exhumation, Curve View, and Text Editor. The first item is the 2D inverse thermal modelling program, while the other two items are data exploration tools allowing you to graphically and textually review the output data from the Cooling/Exhumation algorithm. Future versions of **4DTHERM** will include a range of 1D, 2D and 3D models and other data exploration tools to support 2D/3D dynamic modeling and visualization of magmatic cooling, reconstruction of thermal/exhumation history and (U-Th)/He thermochronology.

Cooling/Exhumation

Open a Cooling/Exhumation Model window for modeling the cooling and exhumation history of igneous intrusions constrained by Geo-/thermochronology data. See Section 5 “Cooling / Exhumation Model” for details.

Cooling Curve Viewer

Open a Curve Viewer window for displaying and comparing up to 10 cooling curves. For details, see Section 6.1 “Curve Viewer Window”. It shows the summary of key modeling information and plots cooling curves with key points marked, plots cooling-rate curves and histograms of the temperature dropped over a given time interval.

Text Editor

Open a blank text editor, same as New in the Menu Bar. See Section 6.2.

4.2.3. Options Menu

This menu contains a list of functions for changing the appearance and layout of the GUI as well as changing the settings of the model.

Background Color

Change the background color of the current modeling window through the "Change Background Color" dialog box.

Foreground Color

Change the foreground color of the current modeling window through the "Change Foreground Color" dialog box.

Control Panel Color

Change the color of the Control Panel of the current modeling window through the "Change Control Panel Color" dialog box.

Show Legend Panel

A check box indicating whether or not to display the Legend Panel.

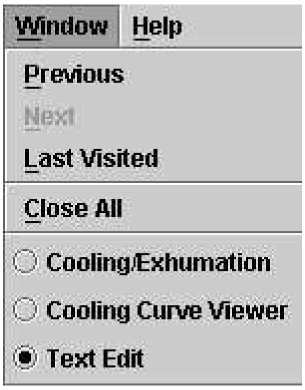
Parameter Settings

Open a small panel for changing the model domain/resolution and modifying values for various parameters. See Section 5.5.1 "Parameter Setting Panel" for details.

GUI Appearance

Open a small panel for changing the "Look and Feel" GUI appearance of the software. Currently only three kinds of "Look and Feel" (Metal, Windows, and Motif), are supported. The default GUI appearance is Metal "Look and Feel".

4.2.4. Window Menu



Contains a list of menu items for manipulating the displaying sequence of the opened modeling windows. All currently-opened windows are listed in the lower part of the menu.

Previous

Display the modeling window that is before the current window. The order of all opened windows is listed in the lowest part of the Options Menu.

Next

Display the modeling window that is after the current window in the window tabs.

Last Visited

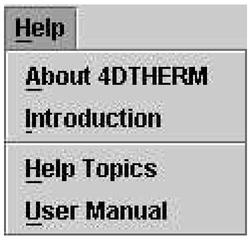
Display the last visited modeling window if it is still opened.

Close All

Close all opened modeling windows. Same as the "Close All" menu item in the File Menu.

4.2.5. Help Menu

About 4DTHERM



Show software information about **4DTHERM** *1.2* and disclaimer.

Introduction

Open a window and show the "Introduction to **4DTHERM**" in an animation running mode. The contents to be displayed in the window include a summary of main features of the GUI, a list of 2D/3D models and the main functions supported, and a brief introduction to the software development.

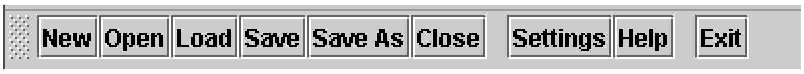
Help Topic

(Not available in this software)

User Manual

Show the Users Manual in html format (not available in this software).

4.3. Toolbar



The Toolbar is also on the top of the interface and is just below the Menu Bar. It contains a set of menu buttons that are the shortcuts of those most-often-used menu items in the Menu Bar. So, all menu buttons on the Toolbar perform the same functions as the corresponding menu items but are accessed in a more convenient way.

New

Open a new (blank) text document for creating/editing input data files. Same as the "New" menu item in the File Menu.

Open

Open an existing ASCII text file for viewing or editing. Same as the "Open" menu item in the File Menu.

Load

Load data (either raw data or resultant data) from a formatted ASCII text file into a model for processing. Same as the "Load" menu item in the File Menu.

Close

Close the currently-visualized modeling window. Same as the "Close" menu item in the File Menu.

Save

Save the modeling results, including all initial settings, into a selected file. Same as the "Save" menu item in the File Menu.

Save As

Save the modeling results, including all initial settings, into a new file with a specific file name. Same as the "Save As" menu item in the File Menu.

Settings

Open a small panel for changing the model domain/resolution and modifying values for various parameters. Same as "Parameter Settings" in the Options Menu.

Help

Show the help topic. Same as the “Help Topic” menu item in the Help Menu.

Exit

Exit the software. Same as the “Exit” menu item in the File Menu.

4.4. Status Bar

The Status Bar is located at the bottom of the user interface and consists of a Message Board and a CPU Running Timer. The Message Board is a text field which cannot be edited. It displays the current status of the model or instant messages about an operation being performed. When running a cooling process, it displays step-by-step cooling states of the *Key Sample*, e.g., current geologic time in Ma, the temperature, depth and cooling rate of the *Key Sample*, etc. It also shows error and warning messages on illegal operations and invalid inputs. Whenever such an error/warning message occurs, the Message Board will be highlighted in red color.

The CPU Running Timer displays the duration of an operation in red color, and a currently-running process or procedure. Please note that it does not display how long the software has been running or how long a model window has been open. It displays, for example, how long the software takes to load data from a file. More often, it is used to record the total time that a modeling process has been running. Pressing the “Reset” button in the Control Panel will reset the Timer. The time displayed in the Timer window is in the format of “hhh:mm:ss.sss” and will be updated at each single operation or after each iterative computation on all elements and nodes of the model.

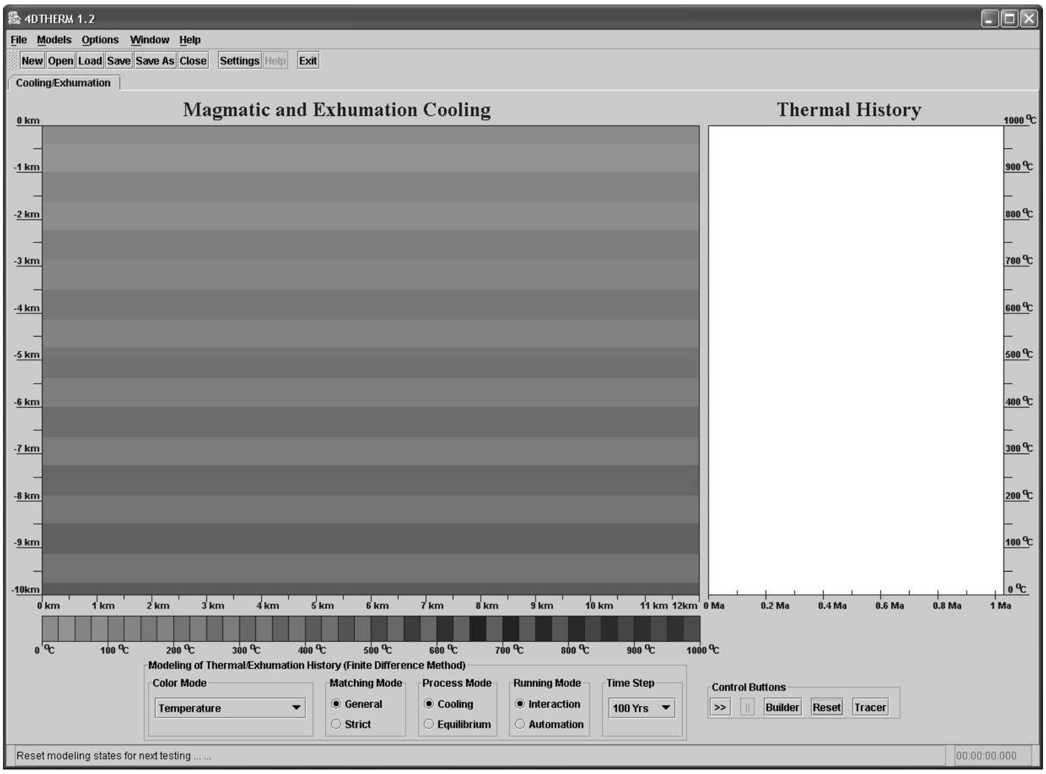
Tips:

a) Always observe the messages displayed in the Status Bar because these message include not only the current running status of a processing, but also the warning messages on illegal operations, error information on invalid inputs and clues for next operation, etc.

b) If the message is too large to be fully displayed in the Message Board, use the mouse to drag the text in the board until the hidden portion of the message can been seen.

5. Cooling/Exhumation Model

The Cooling/Exhumation Model is the main 2D thermal model in this software. It inversely models the geo-/thermochronometry data to reconstruct the thermal and exhumation history of an igneous intrusion. Besides the Menu Bar, Toolbar and Status Bar that we have already introduced in the previous section, the Cooling/Exhumation Model consists of a Viewing Window, a History Window, a Legend Panel, and a Control Panel.



The layout of the Cooling/Exhumation Model. The large color window on the left is the Viewing Window which displays the distribution of temperature in the vertical cross section. The white window on the right is the Thermal History Window on which the modeled cooling curves for samples are plotted and age data points are drawn. Below the two windows are the Legend Panel and Control Panel.

Right-clicking on the Viewing Window, the History Window, or the Legend Panel will open a popup menu which contains a set of shortcuts for controlling the color and visibilities of some GUI components. These shortcuts are self-explanatory and will not be explained in the manual.

5.1. Viewing Window

The Viewing Window shows the distribution of temperature or lithology in the 2D vertical cross section. It has a vertical Depth Scale and a horizontal Distance Scale. The Depth Scale starts from 0 m at the top and increases downward to 10,000m at the bottom. The horizontal Distance Scale shows the relative distance with respect to the left boundary of the model domain and the distance increases from left to right. The lengths of both scales can be adjusted by changing the values in the “Model Height” text filed and/or the “Model Width” text field in the Parameter Setting Panel (see Section 5.5.1), respectively.

The upper-left corner of the window displays the number of steps the cooling process has run, and the corresponding age in Ma is displayed at the upper-right corner of the window (Fig. 5-3). The start step is 0 and the start age is the emplacement time which is extrapolated from the zircon U/Pb age of the *Key Sample*.

There are three color-displaying modes that the software supports: Temperature Color Mode, Lithology Color Mode, and Accumulated Time Mode. The “Color Mode” combo box in the Control Panel controls the switches between the three modes.

Temperature Color Mode

In this color mode, the distribution of temperature in the cross section is displayed in the Viewing Window. As shown in the image above, each color band represents an isotherm of 25 ºC.

Lithology Color Mode

Under this mode, the distribution of all lithologies constructed in the model is displayed in the vertical section.

Accumulated Time Color Mode

Under this mode, the Viewing Window will display the distribution of accumulated time during which the temperature of an element falls in a particular temperature interval since emplacement. This temperature interval may be important to a specific study. For example, the default temperature interval is 300-500 ºC between which it is believed that most copper mineralization occurs.

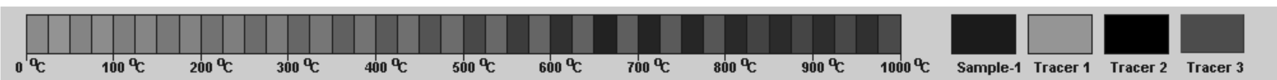
5.2. Thermal History Window

The Thermal History Window is on the right side of the interface. It also has two scales: Temperature Scale and Time Scale. The vertical Temperature Scale starts from 1000 ºC at the top and decreases downward to 0 ºC at the bottom. The Temperature Scale can be changed by changing the value of the “Highest Temp” text filed in the Parameter Setting Panel. The minimum range of the Temperature Scale is 1000 ºC. For example, if the highest temperature is reduced to 800 ºC through the Parameter Setting Panel, the vertical Temperature Scale still ranges from 0 to 1000 ºC.

The Time Scale is at the bottom. It starts from 0 on the left and increases rightward to 1 My on the right. More conveniently, the length of the Time Scale can be easily changed by mouse-dragging over the Time Scale. The minimum time length is 0.01 My.

Upon loading age data into the model, the length of the Time Scale will be automatically adjusted to accommodate all age data from samples. A subtitle of the igneous body studied is shown on the left-top corner of the window. All age data are drawn in small circles at the corresponding position in the window, each of which is pointed by an arrowed data box which contains the name of the dating method and the corresponding age. When running the cooling process, the temperature-time cooling curves of all samples and defined tracers are plotted in different colors in the window.

5.3. Legend Panel



The Legend Panel consists of two kinds of legends: Variable Legends (on the left) and

Sample/Tracer Legends (on the right). Colors for all legends can be changed. See 5.6.3 "How to change a legend's color".

Sample/Tracer Legends

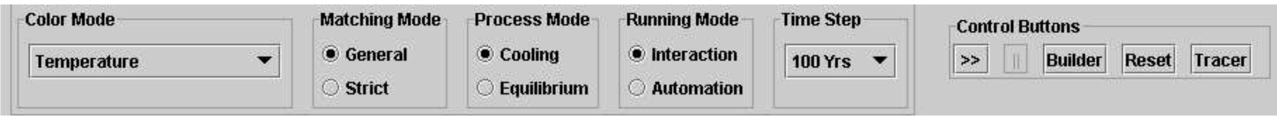
Legends for both samples and tracers are displayed together because a sample is a special tracer. The Sample/Tracer Legends are on the left part of the panel, just below the History Window. They are separate rectangles filled with assigned colors. The color assigned to each sample/tracer is consistent between the Viewing Window and the cooling curve in the History Window.

Variable Legends

The Variable Legends are always under the Viewing Window. They show a series of values for a given variable and the distribution of this variable is displayed in the Viewing Window. In consistent with the three color-displaying modes in the Control Panel, there are also three kinds of variable legends: Temperature Legends, Lithology Legends, and Accumulated Time Legends.

- **Temperature Legends**
  Consist of 40 rectangular legends and legend colors which grade gradually from greenish for low temperature to reddish or purplish for high temperature. The temperature range of the legends is fixed between 0 to 1000 ºC. Therefore, each legend represents an isotherm of 25 ºC. Temperature <= 0 ºC is drawn in white color while >1000 ºC is drawn in red color.
- **Lithology Legends**
  The Lithology Legends contains legends for all lithologies constructed in the Viewing Window.
- **Accumulated Time Legends**
  The Accumulated Time Legends consist of 42 rectangular legends. Each legend represents 5 Ky of time length. If the accumulated time is 0, then the legend's color is white.

5.4. Control Panel



The Control Panel contains a set of control buttons, radio buttons and combo boxes. We are going to introduce all of them from the left to the right.

Color Mode Combo Box

There are three choices of color-display: Temperature Color Mode, Lithology Color Mode, and Accumulated Time Mode. To choose a color mode, click the "Color Mode" combo box, and select one of the three choices. If the color mode is changed, the vertical cross section in the Viewing Window will display the colors of a variable with respect to the new color mode (see Section 5.1 Viewing Window), and the Variable Legends in the Legend Panel will be changed accordingly (see Section 5.3 "Legend Panel").

Matching Mode Radio Button Group

This button group includes both the General and Strict radio buttons. They are used to indicate a flag of the matching mode which is used by the matching routine to assess whether a cooling process has been successful at the end of a testing. If the "General" radio button is toggled, the criteria used to identify a match is less stringent; if the "Strict" radio button is toggled, then the matching routine will use a strict matching criteria. The default matching mode is General. For how the match-checking procedure works, see Section 5.6.4 “How to assess a testing”.

Process Mode Radio Button Group

This button group is used to control which modeling process is going to be run. It consists of two radio buttons: Cooling and Equilibrium.

If the “Cooling” radio box is selected, clicking the “>>” button will run the magmatic and exhumation cooling processes. For how to run the magmatic and exhumation cooling processes, see Section 3.2 “Run the Model”.

If the “Equilibrium” radio box is selected, the “Time Step” combo box, the matching mode radio buttons, the “Builder” button and the “Tracer” button in the Control Panel will be disabled because these GUI components are not in use when running the thermal equilibrium process. With the “Equilibrium” radio box being selected, clicking the “>>” button will run the thermal equilibrium process. For why we need to run and how to run the thermal equilibrium process, see Section 5.6.5 “How to run the thermal equilibrium procedure”.

The default process mode is “Cooling”. The process mode cannot be changed if the model is running or the initial model states have been changed. In this case, you have to press the “Reset” button to re-initialize the model states before changing the process mode.

(***Warning***: *pressing the “Reset” button will clear all constructed igneous bodies, defined tracers, cooling curves and modeling results, regardless of whether the results have been saved or not*).

Running Mode Radio Button Group

This button group consists of two radio buttons: Interaction and Automation. If the Interaction radio button is toggled on, the cooling process will run one step at <u>each</u> clicking of the “>>” button. If the Automation radio button is toggled on, the cooling process will be running continuously after clicking the “>>” button once. The default running mode is Interaction. Press the “Reset” button and the running mode will automatically change to Interaction mode.

“Time Step” Combo Box

This item contains a list of time lengths ranging from 1.0 year to 1.0 My. The value selected from this combo box is the geological time length to be modeled at each step and at the end of this time length the program will update and render all graphics.

The default time step is 100 years for the first stage of magmatic cooling. In order to reduce the size of the text file to be saved, the length of the time step will be changed automatically by the program to 1Ky if the intrusion has transited to the second stage of magmatic cooling. If the intrusion has cooled down, the length of the time step will be further changed to 2Ky, 5Ky or 10Ky depending on the cooled age. However, the time increment can be changed at any step but, if you click the “Reset” button, it will return to 100 years.

“>>” Button

This is the “Run” button. Click the “>>” button and the program will run a modeling process which is determined by the process mode (see “Process Mode Radio Button Group”). If the process mode is “Cooling”, the model will run the magmatic and exhumation cooling processes. If the process mode is “Equilibrium”, the model will run the thermal equilibrium procedure.

If you want to run the modeling process automatically, select the “*Automation*” radio button and then click the “>>” button. In this case, the “>>” button will be disabled. This button will also be disabled if the testing has finished no matter what running mode it is in. Clicking the “Reset” button will enable this button again.

“||” Pause Button

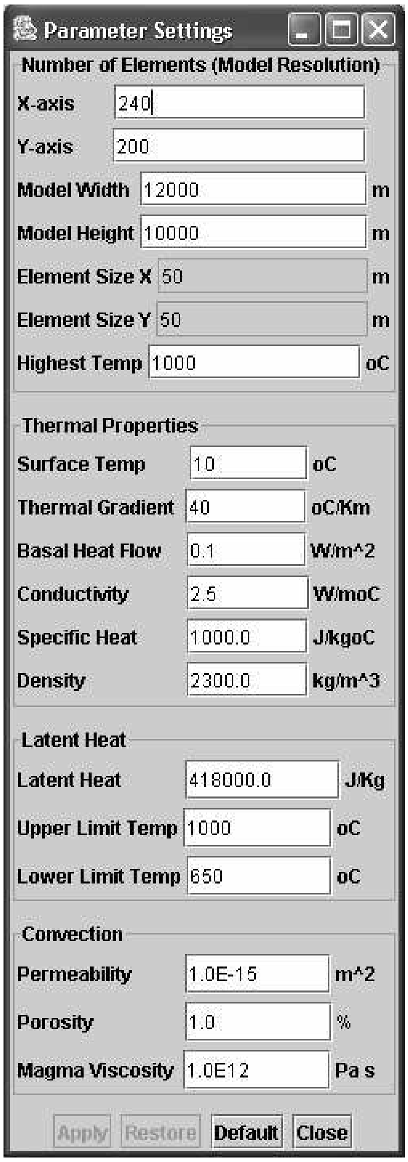
Click the “||” button and the modeling process will be paused.

“Builder” Button

This button is used to open a Geobody Building Panel (see Section 5.5.2). To open a Geobody Building Panel, you must first load age data. Otherwise, this panel cannot be opened.

“Reset” Button

The “Reset” button is used to reset the modeling state and re-initialize all parameters for the next testing run. **Special caution must be taken before pressing this button!** It will clear all constructed igneous bodies, defined tracers, cooling curves and modeling results**, regardless of whether the results have been saved or not**. If the model is running when you click the “Reset” button, an Information Dialog Box will pop up to inform you that you “Cannot reset the model while it is running”. So, if you want to reset the model, you have to stop the running process by pressing the pause button “||”. At any time, only one of the “>>” and “||” buttons is enabled.



“Tracer” Button

This button is used to open a Tracer Defining Panel (see Section 5.5.3).

5.5. Input Panels

5.5.1. Parameter Settings Panel

The Parameter Settings Panel is used as a basic data input facility through which most parameters related to the background of the model can be initialized and modified. It consists of a set of text input fields which are clustered into four groups and a group of buttons.

a) Parameters Related to Model Domain

“X-axis” and “Y-axis” Text Fields

These are used to define the number of elements in both the x-axis and y-axis. The 2D solution domain in **4DTHERM** *1.2* is discretized into a finite number of rectangles which are called elements. Each of these elements has four nodes which defines the shape and position that element. Properties are either assigned to nodes or elements. The default values are 240 elements in the x-axis and 200 in the y-axis.

“Model Width” and “Model Height” Text Fields

These are used to define the width and height of the geological object that the model represents. The default values are 12,000 m wide and 10,000 m high.

“Element Size X” and “Element Size Y” Text Fields

These show the size of an element. Both text fields cannot be edited because their values are determined by the size of the model and number of elements. If any of these values is changed, the element size will be automatically updated.

“Highest Temp” Text Field

This specifies the highest temperature the model can support. The highest temperature defined here is different from the initial temperature of igneous bodies. The later must not be higher than the former. The default value is 1000 ºC.

b) Parameters Related to Thermal Properties of the Default Country Rock

“Surface Temp” Text Field

Defines the surface temperature of the model. The default value is 10 ºC. In **4DTHERM** ***1.2***, the upper boundary condition is set to be “constant surface temperature”.

“Thermal Gradient” Text Field

Defines the initial thermal gradient of the model represents. The default value is 40 ºC/km.

“Basal Heat Flow” Text Field

Defines the basal heat flow of the model. The default value is 0.1 W/m^2. In **4DTHERM** ***1.2***, the lower boundary condition is set to be “constant basal heat flow”.

“Conductivity” Text Field

Specifies the thermal conductivity of the default country rock. The default value is 2.5 W/mºC. The default country rock is always constructed as the background of the model and is different from all other country rocks that are constructed through the Geobody Building Panel.

“Specific Heat” Text Field

Specifies the specific heat of the default country rock. The default value is 1000 J/kgºC.

“Density” Text Field

Specifies the density of the default country rock. The default value is 2300 kg/m^3.

c) Parameters Related to Thermal Properties of Igneous and Country Rock

“Latent Heat” Text Field

Defines the latent heat of crystallization and fusion. The default value is 418,000 J/kg. In **4DTHERM** ***1.2***, the latent heat of crystallization and fusion is assumed to be uniformly released over a range of temperatures which is defined in the next two text fields.

“Upper Limit Temp” Text Field

Defines the upper limit of the temperature range over which latent heat is released. The default value is 1000 ºC. The upper limit temperature defined here must be lower than or equal to the initial temperature of igneous bodies.

“Lower Limit Temp” Text Field

Defines the lower limit of the temperature range over which latent heat is released. The upper limit temperature is the solidus temperature. Its default value is 650 ºC.

d) Parameters Related to Thermal Convection

"Permeability" Text Field

Defines the permeability of all country rocks. The default value is 10^{-15} m^2. If the permeability is set to be 0, then no hydrothermal circulation will occur.

"Porosity" Text Field

Defines the porosity of all country rocks. The default value is 1.0 %.

"Magma Viscosity" Text Field

Specifies the dynamic viscosity of magma. The default value is 10^{12} Pa·s. If the dynamic viscosity of magma is set to be 0, then no thermal convection will occur within the magma.

e) Control Buttons

"Apply" Button

This button is used to enforce all changes made and apply all new values to the model. Its default state is disabled. If any changes are made, this button will be enabled. If changes have been made, this button will be disabled again.

"Restore" Button

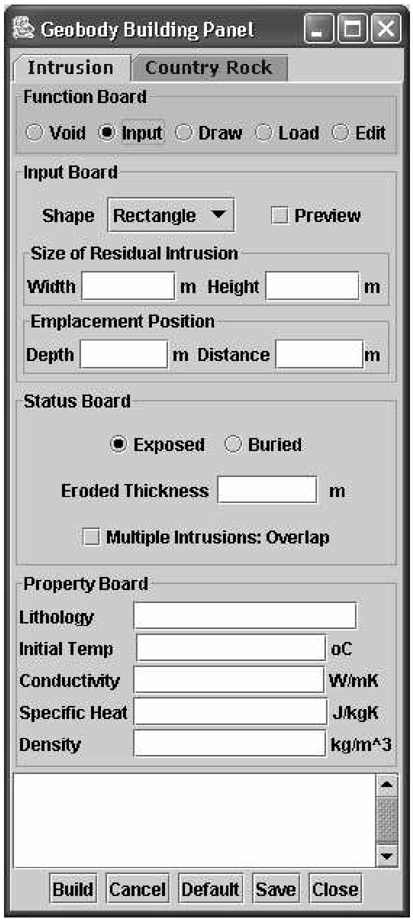
This button is used to restore the previous values to the parameters whose values have been changed but have not been enforced. The default state of this button is disabled. If any changes have made, this button will be enabled. If changes have been enforced, this button will be disabled again.

"Default" Button

This button is used to assign the default values to all parameters. Note that the function of this button is different from the "Restore" button. The latter only restore to the previous values which may be not the same as the default values.

"Close" Button

This button is used to close the Parameter Settings Panel.



5.5.2. Geobody Building Panel

The Geobody Building Panel contains two tabs: Intrusion Tab and Country Rock Tab. Each of them contains a set of text input fields, check boxes, and buttons which are grouped into several boards based on their functionality.

1) Intrusion Tab

This tab is used to construct both regular and irregular shapes of igneous bodies. It consists of seven boards: a Function Board, an Input Board, an Edit Board, a Status Board, a Property Board, an Info Board and a Control Buttons Board.

Note that the Input Board and the Edit Board cannot co-exist and only one of them appears in the panel at any time. If the "Void" or "Input" radio button is toggled on, the Input Board will appear and the Edit Board will disappear. If the “Draw”, “Load” or “Edit” radio button is toggled on, the Input Board will be replaced by the Edit Board.

a) Function Board

It consists of a group of five radio buttons, each of which specifies a method that can be used to define/edit the outline of an igneous body.

- **Void Radio Button**

  This is the default choice which specifies that no method has been chosen. Under the “Void” state, the Input Board and the “Build”, “Cancel”, Default” and “Save” buttons on the Control Buttons Board are disabled. If other radio buttons are toggled on, the Input Board and the four buttons will be enabled.

- **Input Radio Button**

  If the “Input” radio button is toggled on, it indicates that the method to be used to define intrusions is by inputting values into the text fields in the Input Board. Using this method, only regular shapes of intrusions can been built.

- **Draw Radio Button**

  If the “Draw” radio button is toggled on, it indicates that the method to be used to define intrusions is by mouse-drawing on the View Window.

- **Load Radio Button**

  If the “Load” radio button is toggled on, a “Load Data From” dialog box will be opened. After having loaded the geometry definition data from the selected file, the outline of the previously-defined body will be displayed in the Viewing Window. If the data have been successfully loaded, the “Edit” radio button will be automatically toggled on so that the loaded outline can be edited and/or built. If the loading operation is cancelled or failed, it will switch to the “Void” state.

- **Edit Radio Button**

  If the “Edit” radio button is toggled on, the outline defined or loaded can be edited using one of the functions from the Edit Board.

b) Input Board

It contains a set of text fields and a combo box that are used to define regular shapes of intrusions. This board works only when the “Input” radio button on the Function Board is toggled on. Press the “Default” button on the Control Buttons Board and all text fields will be assigned default values which are calculated based on the loaded age data and the size of the intrusion.

- **Shape Combo Box**

  This combo box contains a list of shapes for defining the shape of an igneous body. In the 2D model, there are only two basic shapes: rectangle (cylinder) and ellipse. Circle, square and sheet-like shapes are the special cases of the two shapes. If the shape of the body is defined in the age data input file, after having loaded data from the file, the Shape combo box will display the predefined shape.

- **Preview Check Box**

If the “Preview” check box is selected, the outline of the igneous body defined by the size and position text fields will be displayed in the Viewing Window. However, if any text fields in the Input Board are empty or contain invalid values, an error message will be displayed in the Status Bar and no outline will be drawn. If the box is toggled off, the outline will disappear.

- **“Width” and “Height” Text Fields**

  These two text fields are used to define the residual size of the igneous body. The size text fields are initialized with values from the loaded file.

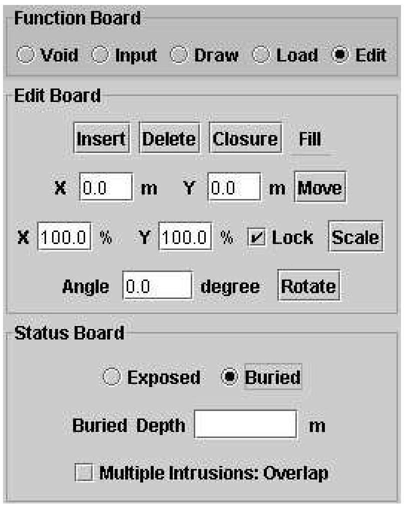
  Note that if the “Exposed” radio button in the Status Board is toggled on, the actual size of the body to be constructed is the sum of the residual size and the amount of igneous rock eroded which is defined in the “Eroded Thickness” text field in the Status Board. If the “Buried” radio button in the Status Board is toggled on, the size defined in the two text fields is the actual size of the body to be constructed.

- **“Depth” and “Distance” Text Fields**

  The “Depth” text field defines the emplacement depth of the igneous body. The emplacement depth should be specified by the user prior to the construction of igneous body. Although a default value is provided based on the loaded age data, there is no guarantee that the testing will succeed.

  The “Distance” text field defines the horizontal distance of the left margin of the igneous body with respect to the left boundary of the model. The default value always puts the body in the middle of the model for the sake of better visualization and reduced computational errors.

c) Edit Board



The Edit Board contains a set of functions that can be used to edit the outline of an intrusion. It appears at the same position as the Input Board when one of the “Draw”, “Load” and “Edit” radio buttons is toggled on. However, this board works only when the “Edit” radio button on the Function Board is toggled on.

- **“Insert” Button**

  This button is used to insert a point at which the mouse clicked into the outline.

- **“Delete” Button**

  This button is used to delete a point selected by the mouse from the outline.

- **“Closure” Button**

  This button is used to close the drawn lines to form a full outline of the igneous body by connecting the first point with the last one. By default, all outlines that are loaded from files or defined by the Input Board are closed.

- **“Fill” Button**

The “Fill” button is used to fill the closed outline with a color. Clicking the “Fill” button, a menu will drop down. The menu contains two choices: “Choose Color” and “No Fill Color”. If the “Choose Color” is chosen, a color palette panel will pop out, and the outline of the intrusion and the “Fill” button will be filled with the selected color. If the drawing is not closed, no color palette panel will pop out. If the “No Fill Color” is chosen, then the outline will not be filled with any color.

- **“Move” Button and “X” and “Y” Text Fields**

  They are used to move the outline of the body around the model. The “X” and “Y” text fields specify the distances to move along x-axis and y-axis, respectively. The “Move” button is used to do the moving action.

- **“Scale” Button, “X” and “Y” Text Fields and “Lock” Check Box**

  These are used to scale the outline by ratios specified in the “X” and “Y” text fields. The “Lock” check box is used to indicate whether the ratios in both the “X” and “Y” text fields should be locked as the same values. For example, when the “Lock” check box is checked, changing the value of the “X” text field, the value in the “Y” field will automatically update to the same value. If the “Lock” check box is not checked, the ratio values in both text fields can be different.

- **“Angle” Text Field and “Rotate” Button**

  They are used to rotate the outline of the body by an angle specified in the “Angle” text field. If the angle is positive, it will rotate clockwise, otherwise counter-clockwise.

d) Status Board

It defines the current exposure status of the igneous body.

- **“Exposed” and “Buried” Radio Buttons**

  If the “Exposed” radio button is toggled, the body defined is currently exposed. If the “Buried” button is toggled, the body is still buried.

- **“Eroded” Thickness Text Field**

  The “Eroded Thickness” text field defines the amount of the igneous rock eroded since exposure if the “Exposed” radio button is toggled (see the figure on page 18). If the “Buried” button is toggled, this text field specifies the current burial depth of the body and meanwhile the label for the text field is updated as “Buried Depth” (see the figure on page 20).

  When the emplacement depth is assumed and the “Exposed” radio button is toggled, the eroded thickness of igneous rock is estimated by the internal computational algorithms. However, there is no guarantee that the testing will succeed based on these initial values.

- **“Overlap” Check Box**

  This box is used in the case of multiple intrusion events. If the box is checked, the body defined will be constructed over previous igneous bodies. Otherwise, no new body is allowed to be constructed over the previous igneous bodies.

e) Property Board

It consists of a set of text fields that specify the physical properties of the intrusion.

- **“Lithology” Combo Box**

  Specifies the lithology of the igneous body to be built.

- **“Initial Temp” Text Field**

  Defines the initial temperature of the igneous body. The default value is 1000 ºC.

- **“Conductivity” Text Field**

  Specifies the thermal conductivity of the igneous body. The default value is 3.0 W/mºK.

- **“Specific Heat” Text Field**

  Specifies the specific heat of the igneous body. The default value is 1046 J/kgºK.

- **“Density Text” Field**

  Specifies the density of the igneous body. The default value is 2700 kg/m^3.

f) Info Board

The Info Board consists of only one text field which is not editable. It shows the instant drawing/editing information and the range of the defined outline of the intrusion.

g) Control Buttons Board

It contains a group of buttons that are used to control the building operations.

- **“Build” Button**

  This button is used to build the defined igneous body. After clicking it, the program will first check the validity of all input values. If any errors are found, an error message will be displayed in the Status Bar. If all values are valid, the igneous body is then constructed into the model as displayed on the screen.

- **“Cancel” Button**

  It is used to cancel and clear all drawings and the “Void” button on the Function Board will be toggled on.

- **“Default” Button**

  This button is used to assign the default values to the text fields on both the Input and Property Boards.

- **“Save” Button**

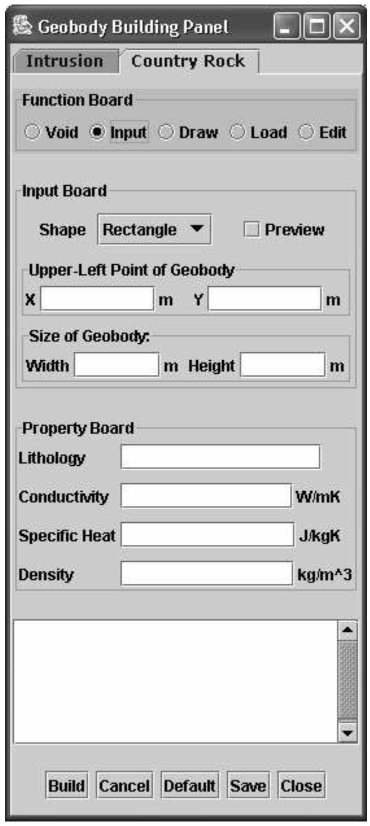
  This button is used to save all drawings (points and lines) and the physical properties into a file.

- **“Close” Button**

  This button is used to close the Geobody Building Panel.

2) Country Rock Tab

This tab is used to construct country rocks of any shapes in the same way as building an intrusion. The reason why not using the same tab to build both the intrusion and country rock is that building a country rock will only change the physical properties at the position delimited by the outline whereas building an intrusion will not only change the properties but also reset the temperature at the portion of the model delimited by the outline to the initial temperature of the magma intrusion.



The Country Rock Tab consists of six boards: a Function Board, an Input Board, an Edit Board, a Property Board, an Info Board and a Control Buttons Board. The Function, Edit, Info and Control Buttons boards are exactly the same as those in the Intrusion Tab, and will not be repeated here. The Input Board and Property Board are very similar to those in the Intrusion Tab except a few differences which will be explained below.

a) Input Board

There are only two differences. First, the "X" and "Y" text fields are used to define the upper-left point of the country rock. These two fields are the same as the "Depth" and "Distance" text fields in the Intrusion Tab except the names are different. Secondly, there are no default values for all text fields in this board. Users are required to input values into these fields to define the country rock if they choose to use the "Input" function.

b) Property Board

It consists of four text fields that specify the physical properties of the country rock to be built. The "Initial Temp" text field is not included in this board as constructing country rock will not reset the temperature. A set of default values are also provided but they are different from those in the Intrusion Tab.

- **"Lithology" Combo Box**

  Specifies the lithology of the country rock to be built. The lithology can be any kind of rocks, including igneous and volcanic rocks.

- **"Conductivity" Text Field**

  Specifies the thermal conductivity of the country rock. The default value is 2.5 W/m^{o}K.

- **"Specific Heat" Text Field**

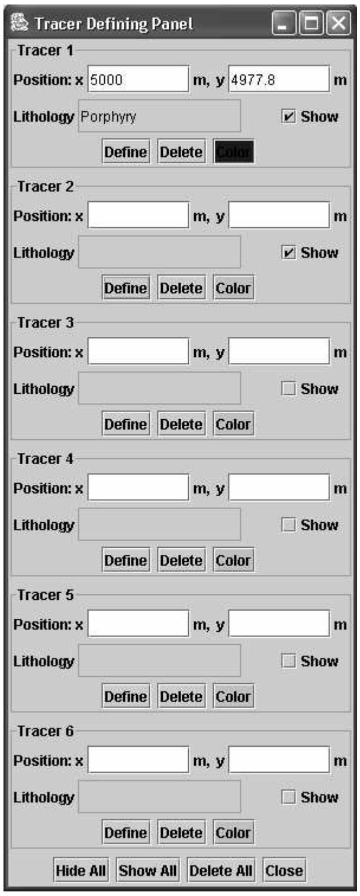
  Specifies the specific heat of the country rock. The default value is 1000 J/kg^{o}K.

- **"Density" Text Field**

  Specifies the density of the country rock. The default value is 2300 kg/m^3.

5.5.3. Tracer Defining Panel

In **4DTHERM**, the modeled cooling profiles of all samples are plotted in the Thermal History window for observation. On occasion, we may want to know the changes in temperature at positions relative to the sample positions. A special monitoring device which is called Tracer is designed in **4DTHERM** to record the changes in temperature, depth, age and many other properties at positions inside the model. The cooling profiles of all tracers are also plotted in the Thermal History window. Using multiple tracers arranged in a specific pattern (e.g., in a vertical and horizontal grid) can maximize the information output in a single run of the model. See Section 5.6.2 for how to define a tracer.



However, cautions should be exercised when defining and utilizing tracers. Only the cooling history of the Key Sample is to be saved and the data outputs for all other tracers/samples are only graphical in nature. The X-Y coordinates of the tracers will be changing as the intrusion approaches to the surface resulting from the erosional exhumation processes. It is the user's responsibility to the keep track of the initial location of the tracer because this information will not be recorded or provided in the output results.

The Tracer Defining Panel is used to define new tracers or to manage and modify the properties of existing tracers. Samples are the most important tracers and their information is also stored in the Tracer Defining Panel. In the Tracer Defining Panel, each tracer has three text fields, one check box and threes buttons:

"Position X" and "Y" Text Fields

These are used to define the initial position of the tracer.

"Lithology" Text Field

This field shows the lithology of the tracer. This text field cannot be edited because the lithology is determined by the position of the tracer.

"Show" Check Box

This check box allows the user to show or to hide the position (in Viewing Window) and the cooling curve (plotted in History Window) of this tracer.

"Define" Button

This button is used to define the tracer. After clicking this button, a tracer mark (small square) will be drawn at the defined position, a legend will be drawn in the Legend Panel, and the lithology of the tracer will be displayed in the "Lithology" text filed.

"Delete" Button

This button is used to delete the defined tracer. Tracers cannot be deleted once the model starts to run.

"Color" Button

This button is used to change the tracer's color. If the tracer is defined, this button will be filled with the legend color. Clicking this button will pop out a "Change Tracer Color" palette panel. Choose a color and click the "OK" button. The color of the tracer is then changed.

4DTHERM *1.2* can support up to six tracers/samples. There are six sets of these text fields and buttons as stated above. At the bottom of the panel, there are four buttons, used to manipulate all defined tracers.

"Hide All" Button

Hides all defined tracers.

"Show All" Button

Displays all defined tracers.

"Delete All" Button

Deletes all defined tracers.

"Close" Button

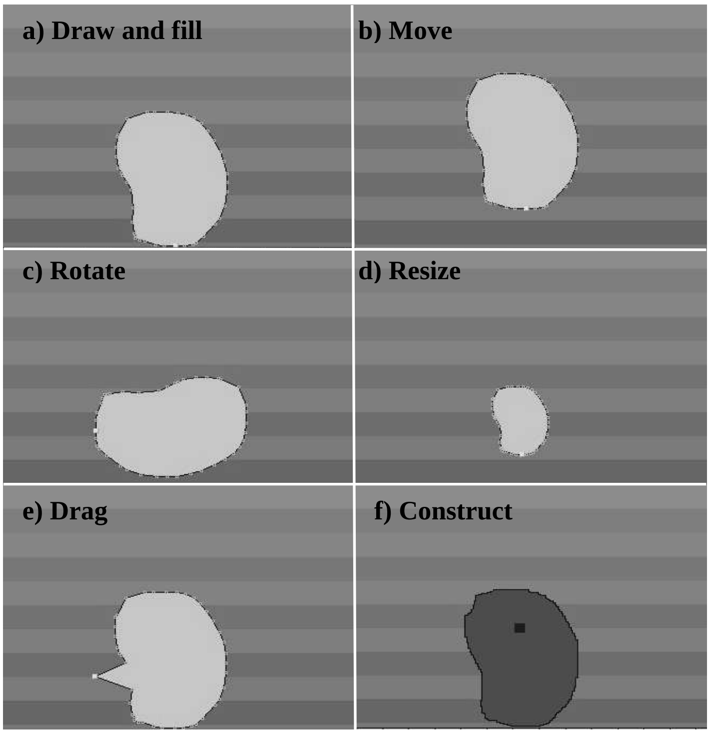
Used to close this panel.

5.6. Functions and Operations

5.6.1. How to Build a Geobody

4DTHERM *1.2* provides the user with the ability to construct both regular and irregular shapes of geobodies, including intrusions and country rocks. However, constructing geobodies into the model must happen after the loading of age data and the initializing of parameter settings.

To build a body, you first have to open a Geobody Building Panel which provides a set of functions to facilitate the task. Choose the appropriate tab for different rocks. Building a body can be done in one of three ways:



Examples showing the construction of an igneous body by mouse drawing. The igneous body drawn on the cross section can be moved (b), rotated (c), resized (d) and dragged (e) through the Geobody Building Panel.

a) Build a body by inputs

Click the "Input" radio button on the Function Board to use the "Input" method. If it is in the Intrusion Tab, click the "Default" button to initialize all parameters with the default values. Change any parameters if needed and assume a value for the emplacement depth. If it is in the Country Rock Tab, you have to choose a shape and input values into all text fields in the Input Board. Click the "Preview" button to preview the position, size and shape of the body in the Viewing Window. You can also edit the defined outline of the geobody using the functions provided in the Edit Board. Click the "Build" button to construct the defined body.

b) Build a body by drawing

Toggle on the "Draw" radio button on the Function Board. Use the mouse to draw the outline of a body on the Viewing Window. After completing the drawing, click the "Closure" button to connect the first point with the last one so that the outline is closed. After the closure, the "Edit" radio button is automatically on. In the "edit" state, you can fill the defined outline with a color by clicking the "Fill" button, and you can delete, insert or drag points, or rotate, move or scale the whole outline to your satisfaction. When finished, click the "Build" button to construct the defined body. If you like, you can click the "Save" button to save the drawn outline into a file so that it can be duplicated for future use by loading it (see below).

c) Build a body by loading

Click the “Load” button to open a “Load Data From” dialog box. Choose a file containing a previously-defined outline of a body. You can also edit the outline as described above. Click the “Build” button to construct the loaded body.

5.6.2. How to Define a Tracer

Tracers are used to record the changes in temperature, depth, age and many other properties at positions inside the model. Defining multiple tracers and arranging them in a specific pattern can maximize the information output in a single effort of testing. New tracers can be defined either by mouse or through the Tracer Defining Panel.

a) Define tracers by mouse

Right click at a position in the Viewing Window where you want to define a tracer and a drop down menu will pop out. Choose “Define This Tracer” from the menu, and then a new tracer is defined. A small square is drawn to mark the position of the new tracer, and new legend is added to the Legend Panel. If you want to move the tracer, use the mouse to drag it around.

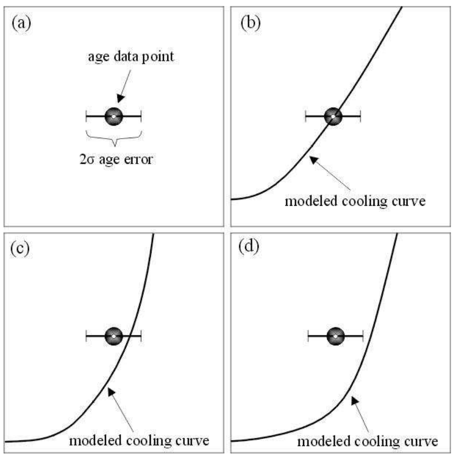
b) Define tracers via Tracer Defining Panel

Click the “Tracer” button in the Control Panel, or right click in the Viewing Window and choose the “Tracer Defining Panel” from the popup menu to open a Tracer Defining Panel. Fill in the “Position X” and “Y” text fields to define the position of the new tracer, and then click the “Define” button to define the tracer.

5.6.3. How to Change a Legend’s Color

To open a color palette panel, double-click a legend or right-click a legend to open a popup menu and then choose “Change Color” from the popup menu. Choose a color and click the “OK” button. Then the legend’s color will be replaced with a new one.

Each legend has a default color. To restore the default color for a legend, right-click the legend to open a popup menu and then choose “Default Color” from the popup menu.



(a) A typical geo-/thermochronometry data is in a format of “age ± σ” where the age units are in Ma. The age data point is shown in a small circle and the corresponding 2σ age error is drawn as a horizontal bar. (b) The modeled cooling curve successfully matches the age data point in **Strict** mode and so does in **General** mode. (c) The modeled cooling curve successfully matches the age data point in **General** mode but fails in **Strict** mode. (d) The modeled cooling curve fails to match the age data point either in **General** mode or in **Strict** mode.

5.6.4. How to Assess a Testing

At the end of each test, a matching procedure checks whether the modeled cooling curve for a sample matches all mineral chronometry age data from that sample. If the resultant curve matches the mineral chronometry data, the test is regarded as successful and the geological setting is physically plausible. If the model fails to match the chronometry data, the test is unsuccessful. The user should iteratively alter the initial conditions until a matching procedure is successful.

There are two standards used to determine whether or not a curve matches a data point. For each age data, the match-checking procedure will work out the corresponding age from the modeled curve. If the difference between the actual age and the modeled age is less than 0.001 My, then the curve is regarded as a match with the age data under the

"*Strict*" matching mode. If the difference is within the range of the 2σ error of the age data but larger than 0.001 My, then the curve matches with the age data under the "*General*" matching mode.

If all age data match the modeled curve under the "*Strict*" mode, the test is regarded as successful. If at least one data matches the curve under the "*General*" mode, and others under the "*Strict*" mode, the test is regarded as successful in the "*General*" mode, but unsuccessful in the "*Strict*" mode. If at least one data does not match the curve under either the "*General*" or the "*Strict*" mode, the test is regarded as unsuccessful.

5.6.5. How to Run Thermal Equilibrium Procedure

In **4DTHERM** *1.2*, it is required that the initial model be in thermal equilibrium prior to the running of the magmatic and exhumation cooling processes. Nonequilibrated initial conditions may result in incorrect "cooled" states and thus introduce some uncertainties or errors to the final modeling results. The thermal equilibrium procedure is implemented based on the "relaxation" technique which has been discussed by Beardsmore and Cull (2001). The essence of the relaxation technique is to ascertain whether each node/element in the model is in a thermal equilibrium with its adjacent neighbours under the initial boundary conditions and thermal properties (Beardsmore and Cull, 2001).

The thermal equilibrium procedure is embedded into the "Cooling/Exhumation" model. To run the procedure, click the "Equilibrium" radio box in the Control Panel of the "Cooling/Exhumation" model, and then click the ">>" button. If the "Equilibrium" radio box cannot be selected, you need to re-initialize the model by clicking the "Reset" button. The running status of the procedure at each step is displayed in the Status Bar, which includes the current thermal gradient, maximum change in temperature and the terminal precision. If the maximum change in temperature is equal to or smaller than the terminal precision, the procedure will stop and the model arrives at a thermal equilibrium state. The terminal precision is set to be 10^{-6} ºC and the precision for the equilibrated thermal gradient can be up to 0.01 ºC/km.

The thermal equilibrium procedure does not simulate the geologic time during which the model reaches a thermal equilibrium state and thus runs very slow. It may take hours to run the procedure before reaching a final thermal equilibrium state for the model. The actual running CPU time of the procedure depends on the difference between the initial thermal gradient and the equilibrated thermal gradient. There are a few tips for saving time in running the procedure. Always observe and make use of the message displayed in the Status Bar. If the maximum change in temperature is 10 times larger than the terminal precision, increase the thermal gradient through the Parameter Setting Panel if the current thermal gradient is increasing or decrease the thermal gradient through if the current thermal gradient is decreasing until the maximum change in temperature is close to the terminal precision. You can do this without stopping the procedure.

The default initial conditions provided are in thermal equilibrium. In addition, for homogeneous model, the initial (pre-intrusion) thermal gradient *dT/dy* can be estimated by Eq 5-1 (Fu et al., 2005):

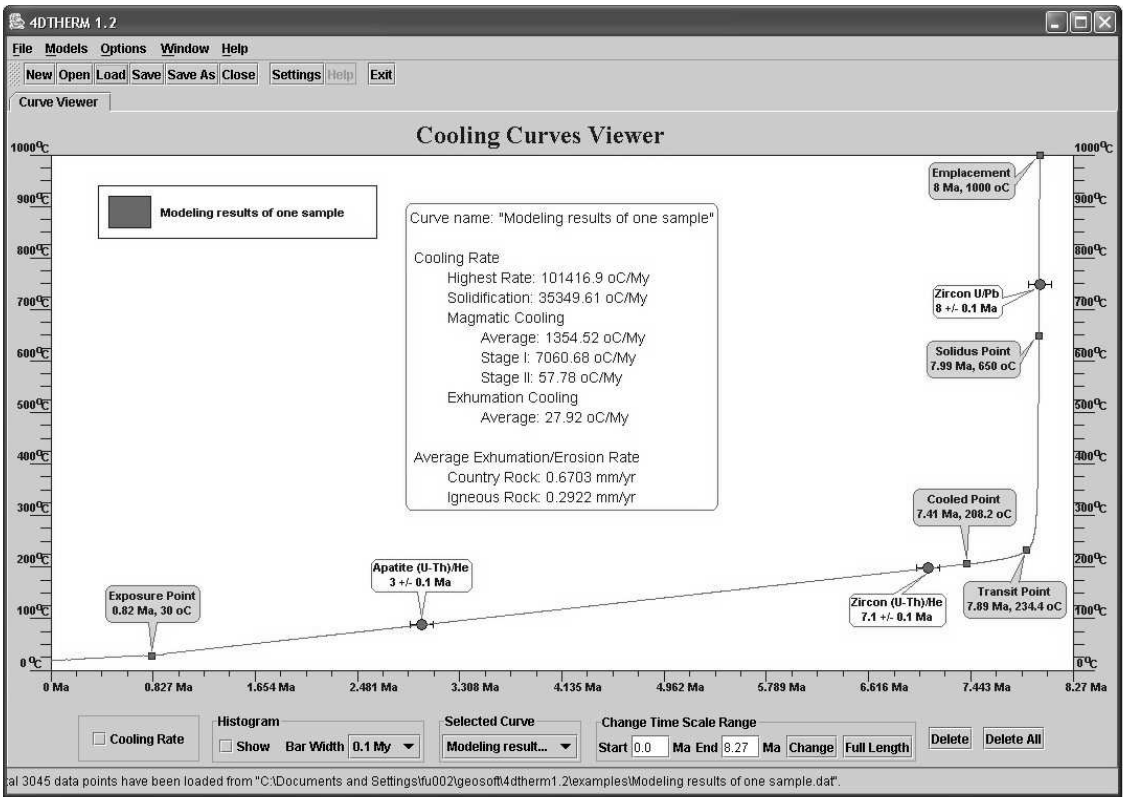
$$\frac{dT}{dy} = \frac{Q_{basal}}{\lambda_{avg}} \qquad 5\text{-}1$$

where Q_{basal} is the basal heat flux and λ_{avg} the average thermal conductivity of the whole model. For instance, if Q_{basal} = 0.065 W/m^2 and λ_{avg} = 2.5 W/mºC, then *dT/dy* = 0.065 / 2.5 = 0.026 ºC/m = 26 ºC/km.

6. Tools

6.1. Cooling Curve Viewer

The Cooling Curve Viewer is a special tool for visualizing the resultant cooling curves produced by **4DTHERM** *1.2*. This data exploration tool allows the user to further study and graphically analyse the saved modeling results which normally contains thousands or millions of bits of data.



The image above shows the typical layout of a Cooling Curve Viewer which includes a graphical Viewing Window and a Control Panel.

6.1.1. Viewing Window

The Viewing Window is used to visualize all modeling results in different methods or formats. It consists of seven parts:

Horizontal Time Scale

The horizontal Time Scale is at the bottom of the window. It starts from 0 on the left and increases in age incrementally to the right. Upon loading a curve, the length of the scale will automatically adjust so that all curves loaded will be displayed in the full length. In addition, the length of the Time Scale can be scaled by changing the values of the “Start” and “End” text fields in the Control Panel or by mouse dragging. Pressing the “Full Screen” button will restore the horizontal axis to its initial setting.

Vertical Temperature and/or Cooling Rate Scales

There are two vertical Temperature Scales, one on each side of the window. Both scales start from 1000 ºC at the top and decrease downward to 0 ºC at the bottom. The range of temperature on the scales will be adjusted automatically based on the highest temperature of all curves loaded. If the highest temperature is >1000 ºC, the scales will scale up to that temperature. However, if the highest temperature is <1000 ºC, the scales will remain at the range of 0 ~ 1000 ºC.

The Temperature Scales are used to scale the cooling curve and histogram graphic. However, when the "Cooling Rate" check box is selected and the cooling-rate curve of the selected cooling curve is displayed in the Viewing Window, the vertical scale on the left side will switch to the Cooling Rate Scale which is 100,000 ºC/My at the top and decreases downward to 0 ºC/My at the bottom. The range of the Cooling Rate Scale will be automatically adjusted based on the highest cooling rate of the selected curve.

Legend Box

The legend box is located at the upper-left of the window. It does not appear unless a curve has been loaded. For each loaded cooling curve, a small rectangle filled with a pre-assigned color will be added to the lower part of the legend. The label for each legend is the name of the file loaded. The "Selected Curve" combo box contains the same curve label list as shown in the legend. The curve/file name of the selected curve is also displayed in the Summary Table. The legend box can be moved by mouse-dragging and can be hidden by right-clicking on the window and select "Hide legend box" from the popup menu.

Cooling Curve

The temperature-time cooling curves are drawn for all loaded files in the same colors as the corresponding legends. All age data points used to constrain the cooling curve are marked with small circles and pointed with data boxes which contains the names of the dating methods and corresponding ages and errors. All key points defined in this software such as solidus, transit, cooled, exposure, and present points are highlighted with small squares in the corresponding legend colors and marked by arrowed data boxes which contain the names of the key points and corresponding ages and temperatures. The positions of all data boxes can be adjusted by mouse-dragging. The visibilities of these data boxes can be changed through the popup menu which can be opened by right-clicking on the window.

Summary Table

This table displays the summarized information about the key points for the selected curve only. For more detailed modeling results, users should refer to the saved file. The position of the summary table can be changed by mouse-dragging and it can be hidden by right-clicking on the window and select "Hide summary table" from the popup menu.

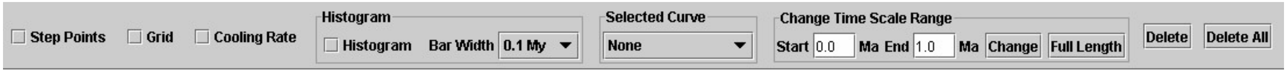
Cooling-Rate Curve

The cooling-rate curve shows the changes in cooling rate with time for a selected cooling curve. The cooling rate is calculated based on the temperature changes over very short time duration and is thus very sensitive to any minor changes in parameters. If the "Cooling Rate" check box is toggled on, the cooling-rate curve of the selected curve will be drawn in the window.

Histogram

The histogram is a graphical representation of the amount of temperature drop over a given time interval. The number occurring above the histogram is the numerical value. The length of the time interval can be adjusted via the "Histogram Bar Width" combo box. If the "Histogram" check box is selected, the histogram of the selected curve will be displayed in the window.

6.1.2. Control Panel



"Step Point" Check Box

The "Step Point" check box is used to indicate whether or not to draw enlarged points for each time step on both the cooling curves and cooling rate curves.

"Grid" Check Box

The Grid check box is used to indicate whether or not to show the horizontal and vertical grids in the Viewing Window.

"Cooling Rate" Check Box

The "Cooling Rate" check box is used to indicate whether or not to show the cooling rate curve of the selected curve. If the selected curve is "None", no cooling rate curve will be displayed even if this check box is on.

"Histogram" Check Box

The "Histogram" check box is used to indicate whether or not to show the histogram of the selected curve. If the selected curve is "None", no histogram graphics will be displayed even if this check box is on.

"Bar Width" Combo Box

The "Bar Width" combo box is used to decide the bar width of the histogram for the selected curve. It contains a list of time lengths ranging from 100 years to 20 My.

"Selected Curve" Combo Box

The "Selected Curve" combo box contains a complete list of curves that have been loaded. It is used to select a curve in order to view more information about that curve. If a curve is selected, the summary table, cooling rate curve (if "Cooling Rate" check box is toggled on) and histogram (if "Histogram" check box is on) and all age data and other critical data points of this selected curve will be displayed in the Viewing Window. If the "None" item in the combo box is selected, only cooling curves and legends of all loaded files will be displayed in the Viewing Window.

If no curves have been loaded or all curves have been deleted, the "Selected Curve" combo box will contain only one choice – "None". If a curve is loaded, it is set to be the selected curve. Accordingly, a legend for this curve will be added to the legend box and its label will also be added into and displayed in the "Selected Curve" combo box.

"Start" and "End" Text Fields

These two text fields are used to control the range of the horizontal Time Scale so that the specified interval of the curves displayed in the Viewing Window can be enlarged. The value of the "Start" field must be smaller than that of the "End" field.

"Change" Button

This button is used to change the range of the horizontal Time Scale which is specified by the "Start" and "End" text fields.

"Full Length" Button

This button is used to display all curves in the full range which is the largest time length of all curves displayed in the Viewing Window.

"Delete" Button

The "Delete" button is used to delete the last loaded curve only. Once a curve is deleted, all curves, summary and legend relate to this curve will disappear, the selected curve will switch to the second last one, and the "Selected Curve" combo box will update accordingly.

"Delete All" Button

The "Delete All" button is used to delete all loaded curves.

6.1.3. Running With Cooling Curve Viewer

1) Open a Cooling Curve Viewer window

Choose "Models" > "Cooling Curve Viewer" from the Menu Bar to open a Cooling Curve Viewer window.

2) Load Data

Click the "Load" button in the Toolbar, or choose "File" > "Load" from the Menu Bar to open a "Load Data From" dialog box. Select a file and click the "Load" button in the dialog box to load the data. Up to 10 cooling curves can be loaded and displayed for comparison.

3) View Cooling Rate Curve

Click the "Selected Curve" combo box to select the curve you want to view if there is more than one cooling curve has been loaded, and then toggle on the "Cooling Rate" check box.

4) View Histogram

Click the "Selected Curve" combo box to select a curve, toggle on the "Histogram" check box, and then adjust the bar width in the "Bar Width" combo box so that all bars of the histogram are clearly displayed.

5) Change the Length of Time Scale

Changing the length of the Time Scale can be done in two ways: a) change the values in the "Start" and "End" text fields and then click the "Change" button, or b) drag the mouse over the Time Scale. If the mouse is on either end of the time scale, dragging the mouse to left/right will increase/decrease the start/end time of the scale. If the mouse is in the middle of the scale, dragging the mouse to either direction will change both the start and end times of the scale and thus will move the whole cooling curve(s) together.

6.2. Text Editor

The Text Editor is an auxiliary tool for creating and editing input data files and viewing output files. Each opened file is displayed in a single window and text editing is done via keyboard. Text-editing functions available to the Text Editor (Select all, Copy, Cut, Paste, Font size) can be accessed by right-clicking the mouse. Note that there is no "Undo" function.

To open a file, click the "Open" button in the Toolbar, or choose "File" > "Open" to open a "Open File" dialog box, then select a file and click "Open" button in the dialog box. To save the changes made for a file, click the "Save" button in the Toolbar, or choose "File" > "Save" from the Menu Bar.

7. Input and Output

7.1. Inputs

Data inputs to the model include: a) size and shape of igneous and country rock units; b) residual sizes and position of igneous bodies; c) age data and corresponding nominal closure temperatures, d) sample position, and e) thermal and physical properties of both igneous and country rock units.

4DTHERM *1.2* supports three data input methods: (a) loading a formatted input file, (b) initializing and modifying parameters via the Parameter Setting Panel, and (c) by constructing geologic bodies through Geobody Builder Panel.

7.1.1. Input File

General Format Rules

In **4DTHERM** *1.2*, although input files are required to follow specified formats, these formats are generally tolerant and flexible. There are however a few general rules that should be followed when composing input files:

- Words after "#" in a line are regarded as comments or remarks and will be ignored by the file parser.
- White space, such as blanks, tabs, and newline characters, are word separators and ignored by the file parser. This means that, if not against the first rule, you can write all text in a single line, or write every term or data in a different line. However, using white spaces to format the structure of the text will increase the readability and elegance of the file.
- Full stop mark "." is reserved for float point number. Hyphen "-" is reserved as negative sign or word connector. All other punctuations are used as word separators and will be ignored by the file parser.
- A term or parameter consisting of more than one word must use the underscore character "_" to connect these words together to form a single word. For example, "Apatite (U-Th)/He" should be written as "Apatite_(U-Th)/He" and "Sar Cheshmeh Cu Deposit, Iran" should be written as "Sar_Cheshmeh_Cu_Deposit_Iran".
- The units for size, distance, and depth are in meters (m), for age in million years (Ma), and for temperature in degrees Celsius (ºC).

Example of an Input File

Bearing these simple rules in mind, we now examine the format of an age data file which is provided with the software for users to test. The contents of the file are shown in Table 1:

Table 1. Example of the age data input file "Age data of one sample.dat"

```
# ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
#                         Age data of one sample.dat
#   This is an example input file which contains age data from one sample
# ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

U-Th-He Age Data                  # Header of the data file

Example_Intrusion_One   1         # Name of Intrusion, Number of Samples
```

```
# Shape,         Width,         Height of the intrusion
Cylinder,         1000,           2000;

# Sample Name, Number of Data, X (horizontal distance), Y (Sample Depth)
# with respect to the upper-left corner of the intrusion
Sample-1,           3,           500.0,         300;

        # Dating Method,        Closure Temp (ºC),   Age (Ma),  2 Sigma Error (Ma)
        Zircon_U/Pb              750                    8.0           0.1
        Zircon_(U-Th)/He         200                    7.1           0.1
        Apatite_(U-Th)/He        90                     3.0           0.1

# ~~~~~~~~~~~~~~~~~~~~~~~~~ End of File ~~~~~~~~~~~~~~~~~~~~~~~~~
```

Explanation of the Example File "Age data of one sample.dat"

The file "Age data of one sample.dat" contains data from a single sample of an intrusion. Lines that begin with # are comment lines that provide structural clarity for novice users.

- The first valid line in the file is the header of the file for it contains the keywords "Age Data". The header indicates what format is specified in the file. **4DTHERM** can support any kind of geo-/thermochronometry data.
- The second valid line "Example_Intrusion_One, 1" shows that the intrusion's name is "Example Intrusion One" and that this intrusion has only one sample.
- The third valid line "Cylinder, 1000, 2000" indicates that the shape of the intrusion is a "Cylinder" with a diameter of 1000 m and height of 2000 m.
- The fourth valid line is "Sample-1, 3, 500, 300" which specifies the sample's name, number of age data available for each sample, and the sample coordinates (X, Y) relative to a location in the igneous intrusion, respectively. Note that in this 2D version of the **4DTHERM** software, the sample's X and Y coordinates are relative to the upper-left corner of the intrusion so that the sample position within the intrusion is fixed no matter what depth the intrusion is constructed.
- The next three valid lines are about the dating methods, nominal closure temperatures, ages and errors of the mineral geo-/thermochronometers obtained from the sample "Sample-1".

The input file specifies all data from one sample of an intrusion. An input file can also contain age data from more than one sample from both the same intrusion and the adjacent country rock. In this case, the second valid line should specify the number of samples available from that intrusion and then the sample position and age data for each sample should be listed in a format as stated above (see another example input file "Age data of two samples.dat").

7.1.2. Initializing Parameters

4DTHERM *1.2* provides a default geologic background with a set of initial parameter values (e.g. surface temperature, thermal gradient, basal heat flow, lithology, thermal conductivity, specific heat, and density, etc.). These parameters can be modified and edited using the Parameter Settings Panel. See Section 5.5.1 "Parameter Settings Panel" for how to initialize parameters.

7.1.3. Constructing Geological Bodies

Constructing geological bodies (including igneous and country rocks) directly into the 2D model is another way to input data. Although the input file contains the definition of the body's size and shape, loading data from it will not result in the construction of the body. These data are sent to the Geobody Building Panel to help define the body. The actual construction of the body is achieved via the "Geobody Building Panel" either by inputting data, by mouse drawing, or by loading predefined outline of the body. See Section 5.6.1 "How to build a geobody" for full details.

7.2. Outputs

The outputs available after each successful test include: a) digitized cooling curves with highlighted key points, (b) parameters calculated during the modeling run such as depth and timing of emplacement of the intrusion, cooling rates of different stages, exhumation/erosion rates for country rocks and igneous rocks, eroded thicknesses of intrusions, and "cooled" and exposure time if the sample was exposed to surface, and c) detailed step-by-step modeling states.

7.2.1. Output File

Modeling results can be saved in a text file at the end of each successful testing. There are no strict format requirements for the output file. Normally, a resultant file is a summary of all parameter setting and modeling results which are grouped into six parts (Table 2). The first four parts are about the initial settings of the model domain, properties of both igneous rock and country rock, and age data. The fifth part is the summary of all modeling results. The step-by-step modeling details are listed in Part 6 for further examination. This part usually contains thousands of or even millions of pieces data. It can be time consuming for users to examine this data manually, and it is recommended that the Cooling Curve Viewer tool should be used to reconstruct and analyse the cooling profile.

Table 2. Example of an output file produced by 4DTHERM *1.2* and the age data are from the file "Age data of one sample.dat" (see Table 1).

#***

 # 4DTHERM *1.2*: Sept. 30, 2005,   Total CPU time: 00:46:31.394

#***

1. General Settings

Model domain: width=12000.0 m, height=10000.0 m

Number of elements: x=240, y=200

Element size: x=50.0 m, y=50.0 m

Surface temperature=10.0 ºC

Thermal gradient=40.0 ºC/km

Basal heat flow=0.1 W/m^2

Latent heat of Crystallization and fusion=418000.0 J/kg

Temperature range of Crystallization and fusion: 650.0 ~ 1000.0 ºC

2. Country Rocks

Lithology="Sediments"

Conductivity=2.5 J/mºC

Specific heat=1000.0 J/kgoC
Density=2300.0 kg/m^3
Permeability=1.0E-15 m^2
Porosity=1.0 %

3. Magma Intrusions

Lithology="Igneous Rock"
Initial emplacement temperature=1000.0 ºC
Conductivity=3.0 J/mºC
Specific heat=1046.0 J/kgºC
Density=2700.0 kg/m^3
Dynamic viscosity=1.0E12 Pa.s
Expansion coefficient of magma=2.0E-5 /ºC
Shape="Rectangle"
Width=1000 m, Height=2000 m
Sample Depth=300.0 m

4. Age Data

Sample No.: Sample-1
Apatite (U-Th)/He: Closure Temperature=90.0 ºC Age=3.0 +/- 0.1 Ma
Zircon (U-Th)/He: Closure Temperature=200.0 ºC Age=7.1 +/- 0.1 Ma
Zircon U/Pb: Closure Temperature=750.0 ºC Age=8.0 +/- 0.1 Ma

5. Summary of Modeling Results

Testing finished successfully in GENERAL matching mode.
The modeled cooling curve matches all age data.
Emplacement Depth=4800.0 m
Emplacement Time=8.003 Ma
Transit Step=1084
Transit time=7.8946 Ma
Cooled Step=1561
Cooled time=7.4176 Ma
Cooled temp of Sample-1=207.1 ºC
Exposed Step=2880
Exposed time=0.8226 Ma
Average cooling rate=124.95 ºC/My
Stage I=7060.68 ºC/My
Stage II=57.78 ºC/My
Magmatic cooling rate=1354.52 ºC/My
Exhumation cooling rate=27.92 ºC/My
500~300 ºC Interval=7.9901 ~ 7.973 Ma
Duration=0.02 My.
Cooling Rate=11714.1 ºC/My.
Average exhumation rate=0.6315 mm/yr

Rate for country rock=0.6703 mm/yr
Rate for intrusion itself=0.2922 mm/yr
Estimated eroded thickness of intrusion=240.3758 m
Magma convection within the igneous body
Start time=8.00285 Ma
End time=7.99565 Ma
Hydrothermal circulation induced by the intrusion
Start time=8.00285 Ma
End time=7.41755 Ma

6. Detailed Step-by-Step Cooling/Exhumation History for Key Sample: "Sample-1"

Total time steps=3045

Step 1: Time=8.0028 Ma; Erosion Rate=0.6703 mm/yr; Sample-1(Temp=1000 ºC, Depth=5349.9 m, Cooling Rate=0 ºC/My); Highest Thermal Gradient=202.02 ºC/km.

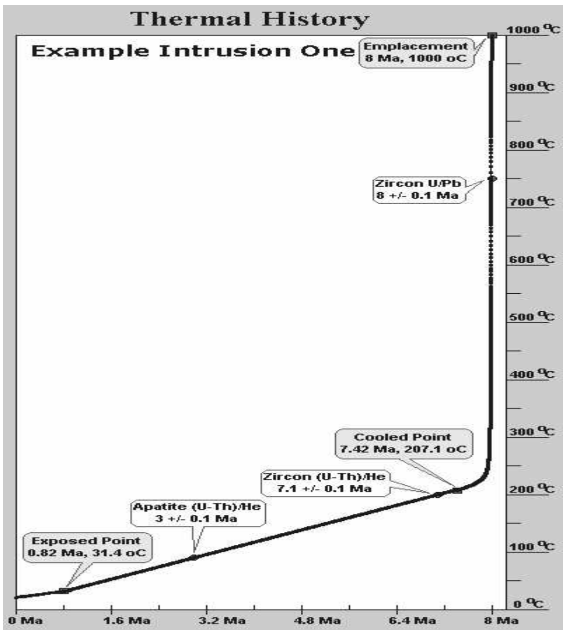
Step 2: Time=8.0028 Ma; Erosion Rate=0.6703 mm/yr; Sample-1(Temp=1000 ºC, Depth=5349.9 m, Cooling Rate=0 ºC/My); Highest Thermal Gradient=202.01 ºC/km.

……

Step 3045: Time=0 Ma; Erosion Rate: (Country Rock=0.6703 mm/yr, igneous rock=0.2922 mm/yr); Sample-1(Temp=20.6 ºC, Depth=308.4 m, Cooling Rate=11.3 ºC/My); Highest Thermal Gradient=39.3 ºC/km.

~~~~~~~~~~~~~~~~~~~~~~~~~~ End of File ~~~~~~~~~~~~~~~~~~~~~~~~~~

7.2.2. Cooling Curve



The cooling curve plotted in the History Window after each successful testing is an important output of this software. The image on the right shows the cooling curve for a successful test where the curve matches all three mineral thermochronology results (small dots). Some critical time points are highlighted by small colored data boxes. Cooling rates, exhumation rates and many other parameters can be calculated based on the digitized cooling curve (see Table 2).

7.2.3. Instant Graphic Output

In addition, the instant visualization of temperature distribution in the vertical cross section at each time step is another valuable output. The graphic output at each time step can be saved manually by pressing "Print Scrn" button on the keyboard and then pasting it to any kind of image/photo editor (e.g., Microsoft Photo Editor in Windows OS; GIMP Image Editor in Linux OS) or Microsoft Word file, etc. If you want to use the saved images to make a PowerPoint presentation or a movie, be sure that these images are cropped into the same sizes.

8. Theory and Algorithms Behind **4DTHERM** *1.2*

I will briefly introduce the computational methods, algorithms and theories employed and developed in **4DTHERM** *1.2* in order to help the users better understand how the program works and what is being computed.

8.1. Governing Equations

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

$$\nabla\left(\rho_f U\right) = 0 \qquad (8\text{-}1)$$

$$U = -\frac{k}{\mu_f}\left(\nabla p + \rho_f g\right) \qquad (8\text{-}2)$$

$$\underbrace{\rho_b C_b \frac{\partial T}{\partial t}}_{\text{heat content}} = \underbrace{\lambda_b \nabla^2 T}_{\text{conduction}} - \underbrace{\nabla\left(\rho_f\ C_f\ U\ T\right)}_{\text{convection}} + Q \qquad (8\text{-}3)$$

where T is temperature, t time, ρ density, C specific heat, λ conductivity, U Darcy velocity, Q internal heat source, p pressure, k permeability, μ dynamic viscosity and g the acceleration of gravity, and subscript f denotes fluid property, and b bulk (rock+fluid) property. Eq. 8-1 represents conservation of mass flow of the fluid, Eq. 8-2 is conservation of momentum expressed by Darcy's law and Eq. 8-3 represents conservation of energy where rock and fluid are assumed to be in local thermal equilibrium at temperature T. The system of equations has been solved using an explicit finite difference scheme.

8.2. Methods of Solutions

8.2.1. Latent Heat of Crystallization/Fusion

In this software, it is assumed that crystallization occurs over a range of temperature between 650 and 1000 ºC and latent heat is uniformly released over this range of temperature within magma bodies. The effect of latent heat is solved at the end of each time step. The final new temperature T'_{n+1} of an element within magma at time t_{n+1} after the release of latent heat is given by (Fu et al., 2005):

$$T'_{n+1} = \frac{T_n \beta + T_{n+1}}{1+\beta} \qquad (8\text{-}4)$$

where T_n is the temperature of the element at time t_n, T_{n+1} the new temperature of the same element at time t_{n+1} after the heat transfer by conduction and convection, β is a factor defined as $\beta = L_m / (C_m\ \Delta T)$, ΔT is the temperature interval of crystallization (ΔT = 1000 – 650 = 350 ºC), L_m the latent heat of crystallization, and C_m the specific heat of magma.

8.2.2. Thermal Convection within Magma Bodies

Thermal convection within a magma body of limited volume is considered as a time-dependent natural convection in a confined domain. It is assumed that magma convection occurs only within a domain where the temperature of magma is above the solidus. As the convection domain within the crystallizing magma body varies with time, the upper and side boundaries are set to be slightly above the solidus temperature (650 ºC), and the lower boundary is set to be at least 100 ºC higher than the upper boundary. The possible size of convection domain and the corresponding thermal Rayleigh number *Ra* are evaluated at each time step. *Ra* is defined by

$$Ra = \frac{g\alpha_v \rho_0 \Delta T d^3}{\mu\kappa} \qquad (8\text{-}5)$$

and the horizontal velocity *u* is given by (Turcotte and Schubert, 2002)

$$u = \frac{\kappa}{d}\left(\frac{Ra}{2\sqrt{\pi}}\right)^{\frac{2}{3}} \frac{\xi^{\frac{7}{3}}}{\left(1+\xi^4\right)^{\frac{2}{3}}} \qquad (8\text{-}6)$$

where g is gravitational acceleration, α_v thermal expansion coefficient of magma, ρ_0 is the density, ΔT is the temperature difference across the convection cell, *d* the cell thickness, μ dynamic viscosity of magma, κ thermal diffusivity of magma, and ξ is the aspect ratio of the convection cell. Convection within the magma is limited within *Ra* of the order 10^3 to 10^6.

8.2.3. Hydrothermal Convection in Porous Rocks

Only the hydrothermal circulation occurring in porous rocks saturated with a single-phase fluid (pure water) are considered in the software. The Rayleigh number *Ra* for hydrothermal circulation in porous media heated from below is defined as:

$$Ra = \frac{g\left(\alpha\rho^2 C\right)_f k d \Delta T}{\mu_f \lambda_r} \qquad (8\text{-}7)$$

where ρ_{f0} is the density of the fluid at temperature T_0 and α_f is the volume coefficient of thermal expansion of the fluid. Hydrothermal convection occurs when the calculated *Ra* reach a critical value of $4\pi^2$. The vertical convection velocity υ is given by (Cathles, 1983; Turcotte and Schubert, 2002):

$$\mathrm{v} = -\frac{k}{\mu_f}\alpha_f \rho_{f_0} g \left(T - T_0\right) \qquad (8\text{-}8)$$

8.2.4. Exhumation/Erosion Cooling

It is assumed that erosional exhumation processes are occurring continuously at the surface since the time of emplacement of the magmatic intrusion. Exhumation/erosion process will not only increase the rate of magmatic cooling but affect the geothermal structure of the model as well. Quantifying this effect is achieved by reducing the temperature of the country rocks by the amount of temperature equivalent to the eroded thickness. The amount of temperature ΔT to be reduced over time Δt due to erosion is calculated by (Fu et al., 2005)

$$\Delta T = v_c \Delta t \ \frac{dT}{dy} \qquad (8\text{-}9)$$

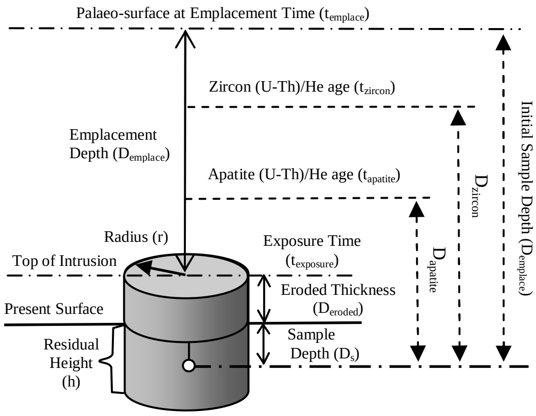
where v_c is the erosion rate, Δt the duration of erosion process and dT/dy the pre-intrusion thermal gradient.

8.3. Inverse Modeling of Thermal and Exhumation History

A complete thermal history of magmatic intrusion includes both the early magmatic-hydrothermal cooling stage and the long duration cooling period associated with erosional exhumation processes. The reconstruction of thermal and exhumation history is achieved in **4DTHERM** *1.2* by the utilization of an inverse modeling algorithm which will be briefly reviewed below.

8.3.1. Calculation of Erosion Rates

The calculation of erosion rates is based principally on U-Th-He thermochronology data and the “cooled” states, and follows the assumption that exhumation and erosion processes have occurred continuously at the surface since the time of intrusion. There are nine different cases in total that may need to be considered, however we briefly review the most general case. For other cases, refer to Fu *et al*. (2005).



Terminology and notations used for calculating the erosion rates of an intrusive igneous body. Refer to Section 8-4 for the definitions of all terminology. (From Fu *et al*., 2005)

Case A: cooled prior to zircon (U-Th)/He age and exposed presently

In this case, the igneous body cooled before its temperature passed through the closure temperature of zircon (U-Th)/He chronometer and the body is currently exposed at the surface. In this situation, both *Zircon (U-Th)/He Depth* (D_{zircon}, for definition, see Section 8.4) and *Apatite (U-Th)/He Depth* ($D_{apatite}$) can be used to calculate the erosion rate. The *Eroded Thickness* of country rock between zircon (U-Th)/He age (t_{zircon}) and apatite (U-Th)/He age ($t_{apatite}$) is ($D_{zircon} - D_{apatite}$), and the erosion rate (v_c) for country rocks is thus determined by

$$v_c = \frac{D_{zircon} - D_{apatite}}{t_{zircon} - t_{apatite}} \qquad (8\text{-}10)$$

The amount of country rock eroded before t_{zircon} is v_c ($t_{emplace} - t_{zircon}$), where $t_{emplace}$ is the *Emplacement Time*. So the *Eroded Thickness* of igneous rock (D_{eroded}) is determined by

$$\mathrm{D}_{\mathrm{eroded}} = v_c\left(t_{emplace} - t_{emplace}\right) + D_{zircon} - D_{sample} - D_{emplace} \qquad (8\text{-}11)$$

which indicates that D_{eroded} is depends on $D_{emplace}$. If we assume a value for the *Emplacement Depth* ($D_{emplace}$), then D_{eroded} is solved and the exposure time ($t_{exposure}$) of the igneous body can also be determined by

$$t_{\text{exposure}} = t_{emplace} - \frac{D_{emplace}}{v_c} \qquad (8\text{-}12)$$

and finally the *Erosion Rate* (v_i) for igneous rock is given by

$$v_i = \frac{D_{eroded}}{t_{\exp osure}} \qquad (8\text{-}13)$$

8.3.2. Inverse Modeling Algorithm

In **4DTHERM** ***v.1.2***, the emplacement depth and eroded thickness of the igneous body is determined through the inverse modeling of all geo-/thermochronometry data utilizing an iterative "trial and error" modeling algorithm.

An emplacement depth is first assumed and then a possible "cooled" state is estimated based on the input data (the size of the intrusion, sample position, geo-/thermochronology data and present exposure/burial status). The model then uses one of the nine algorithms for calculation of a cooling curve. A cooling curve is calculated for the sample in each run of the model. If this cooling curve passes through all of the measured age data points, then this run of the model is considered to be successful (see Section 5.6.4 for how to assess a modeling test), and the assumed emplacement depth and the calculated eroded thickness of igneous rock are "plausible" valid values. The word "plausible" is used here because there are a number of other pairs of emplacement depth and eroded thickness values that can also satisfy the model and result in successful cases. This introduces some uncertainties in the final results. Fortunately, the emplacement depth can be limited to a certain range. Beyond this range, no matter what value of the eroded thickness is taken, the model will fail. Similarly, the eroded thickness can also be limited to a narrow range.

If the testing fails due to the misjudgment of the "cooled" state, the model will automatically adjust the previously estimated "cooled" state and select an appropriate algorithm for the next run of the model. If it fails because of the "incorrect" initial values for emplacement depth and/or eroded thickness of igneous rock, we need to assign new values to both variables, and then run the model again.

8.4. Glossary of Terms used in 4DTHERM *1.2*

Where possible the terminology used in **4DTHERM** *1.2* is consistent with the published literature. A number of new concepts are introduced by the application of the **4DTHERM** *1.2* however, and a glossary is provided below to understand how the terms are defined and used:

Accumulated Time

The Cooling/Exhumation Model can record the time length during which the temperature of an element falls in a particular temperature interval and can display the distribution of this time length in the vertical cross section. The *Accumulated Time* at an element in the model is the total time accumulated during the whole magmatic cooling history when the element's temperature is within the specified temperature interval.

Certain temperature intervals may be important during the cooling of igneous intrusion and can be used as an index for a specific study. For example, it is believed that most copper mineralization may occur at the temperature interval between 300 and 500 ºC (McInnes et al., 2005 and references therein). The default temperature interval is 300-500 ºC, however this interval can be changed through the Parameter Setting Panel (see Section 5.5.1).

Apatite (U-Th)/He Depth

The depth of a *sample* from which apatite (U-Th)/He data is obtained at the time corresponding to the apatite (U-Th)/He age. *Apatite (U-Th)/He Depth* ($D_{apatite}$) is defined by (Fu *et al*., 2005)

$$D_{apatite} = \frac{T_{apatite} - T_s}{dT/dy} \qquad (8\text{-}14)$$

where $T_{apatite}$ is the closure temperature of apatite (U-Th)/He, T_s the surface temperature, and *d*T/*d*y the pre-intrusion thermal gradient. If the *igneous body* is cooled before it passes through the closure temperature of apatite (U-Th)/He, then this depth is the closure depth (Lovera *et al*., 1999) and can be directly used to calculate the erosion rates. Otherwise, it is only a reference depth used to constrain the *Emplacement Depth*.

For example, if we assume the apatite (U-Th)/He age is 1.0 Ma with a closure temperature $T_{apatite}$=90 °C (based on a cooling rate of 10°C/my, Wolf et al. 1996) and the *igneous body* studied is *cooled* before 1.0 Ma, then the depth of the *sample* at 1.0 Ma is given by (8-14):

$$D_{apatite} = \frac{T_{apatite} - T_s}{dT/dy} = \frac{(90-10)}{40} = 2.0\ km$$

assuming T_s = 10 °C and *d*T/*d*y = 40 °C/km. That is to say, under the above conditions, that the *sample* is at a maximum depth of 2.0 km below the surface at 1.0 Ma.

Cooled Time

A critical time when an *igneous body* cools to the same temperature as the surrounding *country rock* assuming normal (pre-intrusion) geothermal gradient conditions, and when both the *igneous body* and *country rocks* reach a final thermal equilibrium state. The corresponding temperature and depth of the *igneous body* at that time is called *Cooled Temperature* and *Cooled Depth*, respectively.

It should be noted that the “cooled” state of an *igneous body* defined above is a relative concept in that it depends on the depth and temperature of the body, pre-intrusion thermal gradient, exhumation rate and many other factors. In implementation, a procedure is designed to check the temperature status of both the *igneous body* and the ambient *country rocks* at each time step. The *igneous body* is regarded as “*cooled*” only if the temperature of any part of the body is the equal or below the pre-intrusion temperature at the same position.

Country Rock / Host Rock

The country rock and host rock are the crustal rock units into which an *igneous body* intrudes. They also include those that are above, beneath or far away from the intrusion studied but within the model domain. *Country Rocks* can be sedimentary rocks, metamorphic rocks, or even volcanic and igneous rocks if these igneous rocks were *cooled* prior to the *emplacement* of the *igneous bodies* studied.

Emplacement Depth

The vertical distance from the palaeo-surface of the studied area to the top of an igneous body at time of *emplacement*. This is not the same as Initial Sample Depth (see below), unless the sample was collected from the uppermost portion of the igneous intrusion.

Emplacement Time

The time when an *igneous body* intrudes into the *country rock* and since that time there has been no obvious movement of magma with respect to the *country rock* (apart from magma convection within the igneous body).

Eroded Thickness of igneous rock

The amount of *igneous rock* eroded since its *exposure*.

Erosion Rate of country rocks

The average *erosion rate* of the *country rocks* above the *igneous body*. This rate may not be applicable to the *country rocks* of the same elevation as the body because the actual constituent of the eroded *country rock* above the body may be unknown. It is assumed that the *country rock* is less competent than the *igneous rock* and therefore will erode at a relatively higher rate.

Erosion Rate of igneous rock

The average *erosion rate* of the *igneous body*.

Exhumation Cooling

A cooling period that starts immediately after the *Cooled time* and is controlled mainly by uplift and erosion processes.

Exposure Time

The time when the top of an *igneous body* reaches to the Earth's surface due to exhumation and erosion processes and the *igneous body* starts to be eroded.

Igneous Body

An igneous intrusion(s) whose thermal and exhumation history is studied by the inverse thermal modelling algorithm in this software. They are assumed to be emplaced in a molten state and at a specific geological time from which the model starts to simulate a thermal history assuming a unidirectional cooling process.

Initial Sample Depth

The vertical distance from the palaeo-surface to the *sample* position. Therefore, by definition, the *Initial Sample Depth* is the sum of the *Emplacement Depth, Sample Depth and Eroded Thickness* of *igneous rock*. The modeled cooling curve of a *sample* is actually controlled by this depth.

Key Sample

When multiple *samples* are used to constrain the thermal history of an *igneous body*, the program will choose a *sample* as the *Key Sample*. Age data from the *Key Sample* is used by the program to estimate a possible "*cooled*" state and to calculate *erosion rates*. The step-by-step message displayed in the Status Bar and the detailed modeling results to be saved are all from the *Key Sample*. Normally, the *Key Sample* (a) is from the *igneous body* studied, (b) contains at least three geo-thermochronology data, and (c) has the deepest *Initial Sample Depth*. If there is only one *sample* available, then this *sample* is by default the *Key Sample* even if it does not satisfy the three conditions.

Magmatic Cooling

The cooling of magma which starts from *emplacement* to the “*cooled*” state. *Magmatic Cooling* is the result of a combined cooling process that includes conductive, convective and exhumation cooling.

Magmatic Cooling, Stage I

The early *magmatic cooling* period starting from *emplacement* to the *Transit Time* is characterized by short duration and very high cooling rate. It is a very important cooling stage during which magmatic convection, magmatic-hydrothermal convection, and the release of latent heat of crystallization occurs.

Magmatic Cooling, Stage II

The late *magmatic cooling* period from the *Transit Time* to the *Cooled Time*. This stage generally spans the time between when the intrusion cooling rate decreases below 200 º C/My and the temperature of the sample is equivalent to the ambient temperature of the adjacent country rock.

Residual Size of an igneous body

The current size of an *igneous body* that is being eroded. Normally we may only know the horizontal size of the body and have limited information about its depth continuity or its original vertical extent.

Sample

A *sample*, in this software, is defined as a rock that has undergone geochronology and thermochronology studies that can be used to constrain the thermal history of *igneous bodies*. The sample may have been obtained from either the Earth’s surface, a drill hole or an underground mine. *Samples* can come from either the *igneous rock* unit itself or from adjacent *country rock* that has been thermally affected by the emplacement of an igneous intrusion. Besides the age data from the *sample*, the spatial position of the *sample* must be known. A *sample*, by default, is a *tracer*.

Sample Depth

The vertical distance from the highest point of an *igneous body* which is currently exposed to the sampling position. If the *igneous ore body* has been mined, then the mined thickness of the *ore body* should be added to the *Sample Depth*. If the *igneous body* is exposed as a topographic high (e.g., a mountain) and the *sample* is obtained from an outcrop which is not the top of the mountain, then the *Sample Depth* is the vertical distance from the top of the mountain to the *sample* position. In particular, if the *igneous body* is not exposed at present, *Sample Depth* is the vertical distance from the present surface of the studied area to the sampling position.

This definition can also apply to *samples* obtained from the ambient *country rocks*.

Tracer

A *Tracer* is a kind of monitoring device used to record the changes in temperature, depth, age and many other properties of a node or an element in the model domain. The cooling profiles of all *tracers* are plotted in the History Window. The position of each *tracer* is indicated by a small square in the Viewing Window and the corresponding legend is shown in the right part of the Legend Panel. Each tracer has its own color to make it distinguished from others, and the color can be changed.

Tracers can be defined in two ways: by mouse clicking or through the Tracer Defining Panel. For details, see “How to define a *tracer*” in Section 5.6.2. By default, all *samples* are *tracers*.

Transit Time

The time around which there is a significant decrease in the cooling rate of an *igneous body*. In the cooling curve, the transit point is the break point in the curve. Based on large number of observations, this point is defined when the cooling rate is less than 200 ºC/My and the difference in cooling rates between two adjacent time steps is less than 2.0 ºC/My.

Zircon (U-Th)/He Depth

The depth of a *sample* at the time corresponding to the zircon (U-Th)/He age. Similarly, *Zircon (U-Th)/He Depth* (D_{zircon}) is defined by (Fu et al., 2005)

$$D_{zircon} = \frac{T_{zircon} - T_s}{dT/dy} \qquad (8\text{-}15)$$

where is T_{zircon} is the closure temperature of zircon (U-Th)/He, T_s the surface temperature, and dT/dy the pre-intrusion thermal gradient. For the meaning and usage of this depth, please refer to *Apatite (U-Th)/He Depth*.

9. Troubleshooting and Feedbacks

As **4DTHERM** *1.2* has not been systemically and intensively tested so far, you may encounter bugs on both the code and runtime computation. If you do, please report them. Your bug reports are valuable contributions to the improvement of **4DTHERM**. However, there is only limited support available for the software and reports may not be promptly answered by the author.

4DTHERM *1.2* is still under development and improvements are constantly being made. You are welcome to provide your feedbacks and/or suggestions on interface appearance, functionality, computational algorithms, improvements, and any other aspects.

Reports of bugs in **4DTHERM** *1.2* and any questions or comments about this software should be sent to the author via qifu6346@mail.usyd.edu.au or fu002@csiro.au.

10. Credit

4DTHERM *1.2* is developed in the hope that it may be useful for scientific research in many areas of geology. It may be used free of charge and may be freely distributed. You are not allowed to profit from the use or distribution of this software in any way. You may, if you like, upload the software to any non-commercial file server with free public access in its original, unchanged form. The author's consent is required to publish or distribute the software on CD-ROM.

Use of this freeware should be credited in research publications and articles as:

Fu, F.Q., 2006. Reconstruction of thermal and exhumation histories of magmatic ore deposits: Inverse modeling of U-Pb-He thermochronology. PhD thesis, School of Geosciences, University of Sydney.

Disclaimer

This software is provided with no warranty, expressed or implied, regarding performance, merchantability, and fitness for any purpose, operation, or data loss. By using this software, you assume all risks and liabilities with regard to any loss arising from the use of **4DTHERM** *1.2*.

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