CONCH: a Visual Basic program for interactive processing of ion-microprobe analytical data

User's Guide

(version: March, 07)

David R. Nelson

Department of Imaging and Applied Physics,
School of Physical Sciences,
Curtin University of Technology,
GPO Box U1987,
Perth, WA, 6001 (Australia)
Tel: +61-8-9266-3736
Fax: +61-8-9266-2377
e-mail: d.nelson@curtin.edu.au

Updated: March 21, 2007

A much-condensed and simplified version of this document was recently published in the Elsevier journal "*Computers and Geosciences*" (a pdf of this publication has been provided with this software). The correct citation for both documents is:

Nelson, D.R. (2006) CONCH: a Visual Basic program for interactive processing of ion-microprobe analytical data. *Computers and Geosciences* 32, 1479-1498.

Table of Contents

List of Tables

List of Figures

About CONCH and this document

CONCH is a computer program coded in Microsoft Excel Visual Basic for Applications, that allows flexible, interactive processing of ion-microprobe geochronology and trace element data. The software runs on both Macintosh and IBM-compatible platforms and will operate most effectively using Excel '97 (Macintosh) or Excel 2000 (Windows). A Linux OpenOffice version is also planned. CONCH uses algorithms applicable to the processing of ion-microprobe data obtained for a wide range of applications.

This software has been specifically designed to aid the comparatively inexperienced User to successfully negotiate the complex task of extracting useable information from SHRIMP (Sensitive High-Resolution Ion MicroProbe) analytical data. The development aims were to automate as many repetitive and tedious tasks as possible, using sensible default but User-editable parameters, yet to provide the User with sufficient information to ensure that data quality can be effectively monitored and to ensure that informed decisions can be made during each data processing step. Operation of the program is comparatively User-friendly and is suited to the non-specialist; common problems encountered in the input data and during data processing are detected and brought to the attention of Users in an informative way. Reports, graphs and tables are generated with limited User intervention, in a consistent style and at publication standard.

This document describes the software, the installation process and its operation. Processing of ion microprobe data is inescapably complex and this task cannot be successfully accomplished without at least a basic level of understanding of many of the underlying concepts involved. This document attempts to provide such a basic level of understanding. It is recommended that this document be read thoroughly before data processing is attempted.

Software Overview

CONCH is a Visual Basic program that enables flexible interactive processing of ion-microprobe data acquired for quantitative trace element, ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr, ^{60}Fe-^{60}Ni and U-Th-Pb geochronology applications. Before reading a data file generated by an ion-probe, CONCH firstly checks many aspects of the input data for consistency; in order to minimize the unintended incorporation of incomplete analyses into the processed data file, CONCH will alert the User if ambiguities are encountered in the input file and processing will not proceed until these are resolved. Default but editable mineral run-tables enable software identification of the secondary-ion species analyzed and for characterization of the standard mineral used. Counts obtained for each species may be displayed in plots against analysis time and edited interactively. Count outliers may also be automatically identified, via a set of editable count-rejection criteria, and displayed for assessment. Background-corrected count rates, ratios and uncertainties are written to a spreadsheet and may be saved as a text-delimited file. Standard analyses are distinguished from Unknowns by matching of the analysis label with a string specified in the Set-up dialog, and processed separately. A report tabulating count rates, ratios, uncertainties for each analysis, and weighted means and uncertainties for Standards and Unknowns separately, can be obtained using a generalized data reduction routine. Specialized routines process trace-element concentration, ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr and ^{60}Fe-^{60}Ni analysis types, and U-Th-Pb isotopic data obtained for zircon, titanite, perovskite, monazite, xenotime and baddeleyite and Th-U disequilibrium analysis types. Correction to measured Pb-isotopic, Pb/U and Pb/Th ratios for the presence of common Pb may be made using the measured ^{204}Pb counts, or the ^{207}Pb or ^{208}Pb counts following subtraction from these of the radiogenic component. Common-Pb corrections may be made automatically, using a (User-specified) common-Pb isotopic composition appropriate for that on the sample surface, or for that incorporated within the mineral at the time of its crystallization, depending on whether the ^{204}Pb count rate determined for the Unknown is substantially higher than the average ^{204}Pb count rate for all session standards. Pb/U inter-element fractionation corrections are determined using an interactive $\log_e$–$\log_e$ plot of common-Pb corrected ^{206}Pb/^{238}U ratios against any nominated fractionation-sensitive species pair (commonly $^{238}U^{16}O^+/^{238}U^+$) for the session standards. Also displayed with this plot are calculated Pb/U and Pb/Th calibration line regression slopes, *y*-intercepts, calibration uncertainties, standard ^{204}Pb- and ^{208}Pb-corrected ^{207}Pb/^{206}Pb dates and other parameters useful for assessment of the calibration-line data. Calibrated data for Unknowns may be automatically grouped according to calculated date and displayed in colour on interactive Wetherill Concordia, Tera-Wasserburg Concordia, Linearized Gaussian ("Probability Paper") and Gaussian-summation probability density diagrams.

Key words: secondary ion mass spectrometry; SIMS; SHRIMP; isotope analysis; Radiometric age; geochronology; data reduction; Visual Basic

System Requirements

CONCH can run on both IBM-compatible and Macintosh platforms. The program operates most effectively with at least 128 Mb of RAM but at least 256 Mb is preferable.

On an IBM-compatible platform, Excel '98 or later is preferable. On a Macintosh, the default version of CONCH requires Excel '97 or later (although it is possible to obtain a version for Excel '95). The Visual Basic package supplied with Macintosh Excel 2000 and later versions are poorly functioning emulator versions of Visual Basic that do not implement well the operation of selected controls on forms. CONCH has been adapted to function with these Visual Basic versions, but its performance is impaired compared with that using Macintosh Excel '97.

Incompatibilities between implementations of the Excel Visual Basic compiler used for Mac OS9/Excel '97 and Windows XP/Office 2000/2003 configurations, have recently (March 2007) been encountered. An error message generated by Excel that (inaccurately) indicates that CONCH has been "*repaired*" following an attempt to load CONCH, provides evidence of this problem. To overcome these incompatibilities, two different compiled versions of CONCH are required. If you use Windows XP/Office 2000/3, install the version of CONCH labelled "CONCHXPO2000.xls".

Windows Users: it is advisable to print out this manual to install CONCH, as use of "alt + tab" to switch between Adobe Reader and Excel applications during installation may interrupt the macro setup.

Naming conflicts between Excel Macros in CONCH and Squid *may* be encountered if Squid Add-Ins have been previously installed in Excel. Resolution of such naming conflicts is planned for the near future, so that Squid and CONCH may be used in a complimentary manner.

CONCH Installation

There are two ways to install CONCH, separately described in lists *a* and *b*. below. To fully install CONCH, follow the instructions in list *a*. The installation process might differ slightly for versions of Excel more recent than Excel 2004, which have slightly different dialogs and procedures (thanks Microsoft!). If the installation process is not obvious from the instructions given in list *a* below, then it may be preferable to operate CONCH using the simple (but less convenient) method, described below in list *b*.

A CONCH dialog box stating "Error 53: file not found" may occur if the path name of a selected input or output file is too long or complex. This (Excel) problem may be rectified either by quitting Excel and/or rebooting your computer.

a. To fully install CONCH:

1. Place "CONCH.xls" into the preferred permanent directory/folder. Once installed, Excel will always look for CONCH components within this directory/folder so CONCH should not be moved from this directory/folder. If in the future you wish to upgrade "CONCH", you should simply replace the existing (old) version in this directory/folder with an upgraded version having the same name.

2. Open Microsoft Excel

3. Close any open Excel default spreadsheet windows

4. Select "Open …" from the Excel "Files" menu item and select "CONCH.xls" from its permanent directory/folder. You may need to select "all files" to see "CONCH.xls" in the open dialog. (An error message during the reading of the CONCH.xls file may indicate that the version of Excel installed is not fully optioned to read Visual Basic programs or, if you have Squid installed, may be due to conflicting Macro names, a problem I hope to rectify in future.)

5. Select "Customize" from the Excel "Tools" pull-down menu.

6. Select the "Toolbars" tab on the "Customize" dialog and check the "Worksheet Menu Bar" item

7. Select the "Commands" tab on the "Customize" dialog, scroll down to and select the New Menu" list item in the "Categories" list box

8. Select and drag the "New Menu" box in the "Commands" listbox up to a position between the Window and Help pull-down items on the Excel Menu Bar

9. Select the "Modify Selection" button on the "Customize" dialog and, in the "Name:" textbox, type "CONCH"

10. Select the "Customize" dialog to end the "Modify Selection"

11. In the "Commands" tab on the "Customize" dialog, scroll down to and select the "Macros" list item in the "Categories" list box

12. Select and drag the "Custom Menu Item" box in the "Commands" listbox up to just below the new "CONCH" menu item between the Window and Help pull-down items on the Excel Menu Bar. Release the mouse; if you've positioned it correctly, the "Custom Menu Item" box should appear as a list item in the CONCH Menu bar item.

13. Select the "Modify Selection" button on the "Customize" dialog and, in the "Name:" textbox, type "Run".

14. Select the "Assign Macro" list item in the "Modify Selection" list

15. In the "Assign Macro" dialog, select the Macro "AARunconc" from the list so that it appears in the "Macro Name:" text box and, in the "Macros in:" text box, select "CONCH.xls". Select "OK"

16. Select and drag the "Custom Menu Item" box in the "Commands" listbox up to just below the "Run" item in the new "CONCH" menu item, between the Window and Help pull-down items on the Excel Menu Bar. Release the mouse; if you've positioned it correctly, the "Custom Menu Item" box should appear as a second list item in the CONCH Menu bar item.

17. Select the "Modify Selection" button on the "Customize" dialog and, in the "Name:" textbox, type "Next Analysis".

18. Select the "Assign Macro" list item in the "Modify Selection" list.

19. In the "Assign Macro" dialog, select the Macro "AANext_Anl" from the list so that it appears in the "Macro Name:" text box and, in the "Macros in:" text box, select "CONCH.xls". Select "OK"

20. Select and drag the "Custom Menu Item" box in the "Commands" listbox up to just below the "Run" item in the new "CONCH" menu item, between the Window and Help pull-down items on the Excel Menu Bar. Release the mouse; if you've positioned it correctly, the "Custom Menu Item" box should appear as a third list item in the CONCH Menu bar item.

21. Select the "Modify Selection" button on the "Customize" dialog and, in the "Name:" textbox, type "Previous Analysis".

22. Select the "Assign Macro" list item in the "Modify Selection" list.

23. In the "Assign Macro" dialog, select the Macro "AAPrevious_Anl" from the list so that it appears in the "Macro Name:" text box and, in the "Macros in:" text box, select "CONCH.xls". Select "OK"

24. Select and drag the "Custom Menu Item" box in the "Commands" listbox up to just below the "Run" item in the new "CONCH" menu item, between the Window and Help pull-down items on the Excel Menu Bar. Release the mouse; if you've positioned it correctly, the "Custom Menu Item" box should appear as a fourth list item in the CONCH Menu bar item.

25. Select the "Modify Selection" button on the "Customize" dialog and, in the "Name:" textbox, type "Preferences"

26. Select the "Assign Macro" list item in the "Modify Selection" list.

27. In the "Assign Macro" dialog, select the Macro "AAShowPreferencesDialog" and, in the "Macros in:" text box, select "CONCH.xls". Select "OK"

28. You can Group the list items into 3 separate "Run", "Next" and "Previous", and "Preferences" groups by selecting to highlight "Next", selecting the "Modify Selection" button on the "Customize" dialog and selecting the "Begin a Group" text item in the "Modify Selection" list. This will insert a spacer bar between the "Run" and "Next" list items. You should do the same for the "Preferences" list item so that a spacer bar is inserted between "Previous", and "Preferences".

29. Click on the "Customize" dialog to close the "Modify Selection" list and then close the "Customize" dialog.

30. Now, using the CONCH Menu item in the Excel Menu, select the "Preferences" dialog. Select the correct platform "IBM-compatible" or "Macintosh" and the other settings you prefer. The screen resolution option will determine which Set-up dialog will be called; the low screen resolution option calls a smaller dialog with a few less options. If you retain the check on the "Revert to default plot settings" check box, every time you use CONCH the changes you make to plot sizes, positions within windows and sheets will be reset to their original settings (those that suit my computer; these default settings may not suit yours).

Excel requires that the "Counts Sheet" be visible and active whenever CONCH is run (i.e. whenever "Run" is selected from the CONCH Menu bar), so ensure that you click on the "Counts Sheet" tab along the bottom of the CONCH window to make the "Counts Sheet" visible each time you use CONCH.

b. The quick and simple method of CONCH partial installation may be used to run CONCH subroutines without the convenience of an Excel CONCH Menu. The partially install CONCH by the quick and simple method:

1. Place "CONCH.xls" into the preferred permanent directory/folder. Once installed, Excel will always look for CONCH components within this directory/folder so CONCH should not be moved from this directory/folder. If in the future you wish to upgrade "CONCH", you should simply replace the existing (old) version in this directory/folder with an upgraded version having the same name.

2. Open Microsoft Excel

3. Close any open Excel default spreadsheet windows

4. Select "Open …" from the Excel "Files" menu item and select "CONCH.xls" from its permanent directory/folder. You may need to select "all files" to see "CONCH.xls" in the open dialog. (An error message during the reading of the CONCH.xls file may indicate that the version of Excel installed is not fully optioned to read Visual Basic programs.)

5. Click on the "Counts Sheet" tab along the bottom of the CONCH window to make the "Counts Sheet" visible. Excel requires that the "Counts Sheet" be visible and active whenever CONCH is run (i.e. whenever "Run" is selected from the "Macro" dialog, so ensure that you click on the "Counts Sheet" tab along the bottom of the CONCH window each time you run CONCH.

6. From the Excel "Tools" menu item, select the "Macro" item and the "Macro…" menu sub-item.

7. Select "CONCH.xls" from the "Macro's in:" pull-down list shown on the "Macro" dialog.

8. Select "AAShowPreferencesDialog" from the list shown in the "Macro" dialog. This should result in "AAShowPreferencesDialog" appearing in the "Macro name" textbox.

9. Select "Run" button from the "Macro" dialog. This should result in the appearance of CONCH's Preferences dialog.

10. Adjust the settings in the Preferences dialog to suit your computer and data processing preferences, then click the "Ok" button on the dialog to dismiss the dialog. These settings will apply every time CONCH is run in future until changed.

11. From the Excel "Tools" menu item, select the "Macro" item and the "Macros…" menu sub-item.

12. Select "AAARunConc" from the list shown in the "Macro" dialog. This should result in "AAARunConc" appearing in the "Macro name" textbox.

13. Select "Run" button from the "Macro" dialog. This should initiate CONCH operation and result in the appearance of CONCH's Set-up dialog.

1. Introduction

Ion microprobes are now widely applied to the determination of trace-element concentrations and U-Pb and Th-Pb formation ages of a wide range of minerals (e.g. zircon, monazite, xenotime, titanite, perovskite, baddeleyite and galena). In practice, this technique can generate vast quantities of numerical data that require complex processing in order to obtain useful age information. The secondary ion spectrum formed during ion-microprobe analysis of even chemically simple minerals is commonly highly complex, and will usually include monomers, molecular and multiply charged species. Furthermore, the relative efficiency of emission of secondary ions from the sample during ion-microprobe analysis commonly varies unpredictably during the analysis session, requiring the periodic analysis of standards of known composition in order to correct for this instrumentally induced drift. Data processing therefore usually involves complex calibration and isobaric corrections before the measurements can be converted into a meaningful result. The monitoring and sound interpretation of ion-microprobe data commonly requires a high degree of understanding of a large number of complex parameters, yet a trend is emerging in which non-specialist Users are required to acquire and process ion-microprobe data under relatively little supervision.

CONCH is a computer program coded in Microsoft Excel Visual Basic for Applications, that allows flexible, interactive processing of ion-microprobe geochronology and trace element data. The software runs on both Macintosh and IBM-compatible platforms and will operate most effectively using Excel '97 (Macintosh) or Excel 2000 (Windows). A Linux OpenOffice version is also planned. It uses algorithms applicable to the processing of ion-microprobe data obtained for a wide range of applications.

The development aims were to automate as many repetitive and tedious tasks as possible, using sensible default but User-editable parameters, provide the User with sufficient information to ensure that data quality can be effectively monitored, and ensure that informed decisions can be made during data processing. Operation of the program is comparatively User-friendly and is suited to the non-specialist; common problems encountered in the input data and during data processing are detected and brought to the attention of Users in an informative way. Reports, graphs and tables are generated with limited User intervention, in a consistent style and at publication standard.

The aims of this document are to:

1. describe many of the features of the CONCH application and aspects of the data reduction approach,
2. demonstrate the application of the software to the processing of ion-microprobe zircon, titanite, perovskite, monazite, xenotime and baddeleyite U-Th-Pb, and Th-U disequilibrium analyses to obtain dates for these minerals, and
3. provide Users with a reference manual for CONCH operation.

CONCH can generate processed data reports (as spreadsheets) and output files (as tab-delimited text files) containing automatically or manually edited background-corrected count rates, ratios and uncertainties and may therefore be applied to the processing of secondary-ion mass spectrometry (SIMS) data obtained for a wide variety of applications. However, for the sake of brevity, this manual focuses on geochronological applications of CONCH; only limited discussion of its application to trace element, Th-U disequilibruim or short-lived nuclide determinations has been included herein.

The latest version of the program, installation instructions and sample input files may be downloaded from http://conch.perthshrimp.com.

Please don't hesitate to contact DR Nelson (d.nelson@curtin.edu.au, Skype name: "DavidRNelson") if you require any assistance in installation and use of CONCH and/or if you would like to be included on the email notification list of update postings.

2. Setting CONCH's operation preferences

Before using CONCH, it is necessary to set default operation parameters to suit your computer and processing preferences. This is undertaken using the Preferences dialog (see Fig. 2.1).

Provided the installation instructions have been followed, the Preferences dialog may be summoned from the CONCH pull-down menu item.

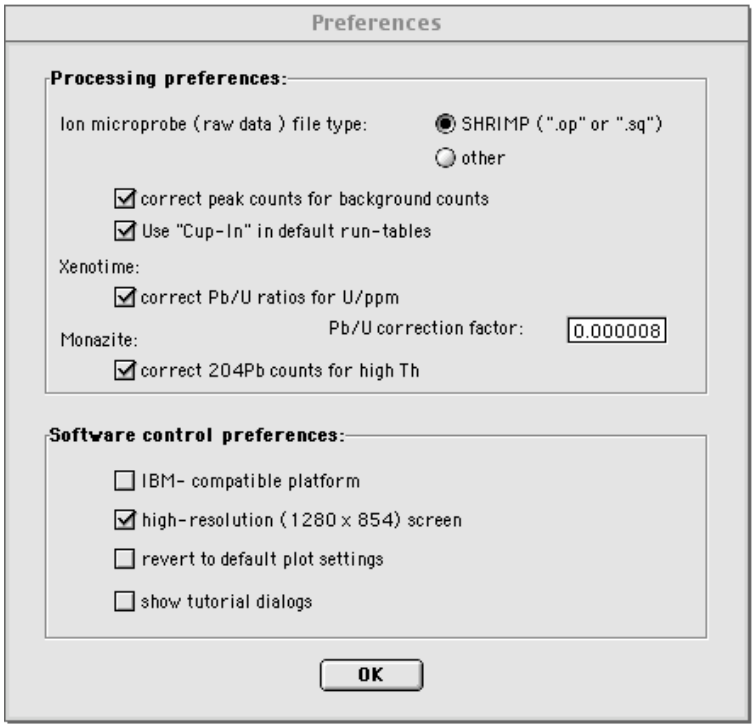

Fig. 2.1. The Preferences dialog.

Table 2.1 lists the controls in the Preferences dialog and describes their functions. CONCH reads the settings in the Preferences dialog every time "run CONCH" is selected (i.e. each time CONCH is run) whether the dialog is summoned or not.

Table 2.1. List of controls in the Preferences dialog, with a description of their functions.

Control label	Control type	Function
Correct peak count for background counts	checkbox	Provided a background species has been specified, subtracts the background count rates for each analysis from the count rates determined for the other species. If not checked, background corrections will not be made.
Use "Cup-In" in default Run-tables	checkbox	If checked, will include "Cup-In" species in the Default run-tables where appropriate (i.e. monazite run-table).
Xenotime: correct Pb/U ratios for U	checkbox	If checked, measured Pb/U ratios will be corrected for high U counts using the method of Fletcher et al. (2000).
xenotime: correct Pb/U ratios for U	editbox	If "Xenotime: correct Pb/U ratios for U" checkbox is checked, uses the U-correction factor read from the editbox and method described by Fletcher et al. (2000) to correct xenotime Pb/U ratios for high U counts
Monazite: correct ^{204}Pb for high Th	checkbox	If checked, uses the method described by Kinny (1997) to correct for excess ^{204}Pb counts of monazite analyses that are attributable to high ^{232}Th count rates
IBM-compatible platform:	checkbox	Adjusts internal settings within CONCH so that software and displays are optimized for Windows versio of Excel Visual Basic. The default settings for the Macintosh platform.
High-resolution (1280 x 854) scree	checkbox	If checked, uses a version of the Set-up dialog that can be displayed on a 1280 x 854 pixel computer display.
Revert to default plot settings	checkbox	uses default plot settngs suited to Macintosh or IBM-compatible platforms and inserts these into the textboxes of the Plot Options dialog
Show tutorial dialogs	checkbox	Displays message boxes with useful information to aid Users of CONCH

3. Input and output file formats

Ion-microprobe output (raw data) files, as well as CONCH-processed data files in several different formats, may be read directly by CONCH. Examples of some of the file formats readable and output by CONCH are provided in the "example input files" folder supplied with CONCH (see Appendix 1). All processing control parameters are assigned sensible default values but these are editable, via a Set-up dialog (see Fig. 3.1, 3.2), prior to reading the input data file. SHRIMP output files may be read using default run-tables for zircon, titanite, perovskite, monazite, xenotime, baddeleyite and Th/U disequilibrium analysis types. There are two versions of the Set-up dialog; each is suited to display on computer screens of different resolution (set in the Preferences dialog). Functions of all controls in the Set-up dialogs are described in Tables 3.1 to 3.6.

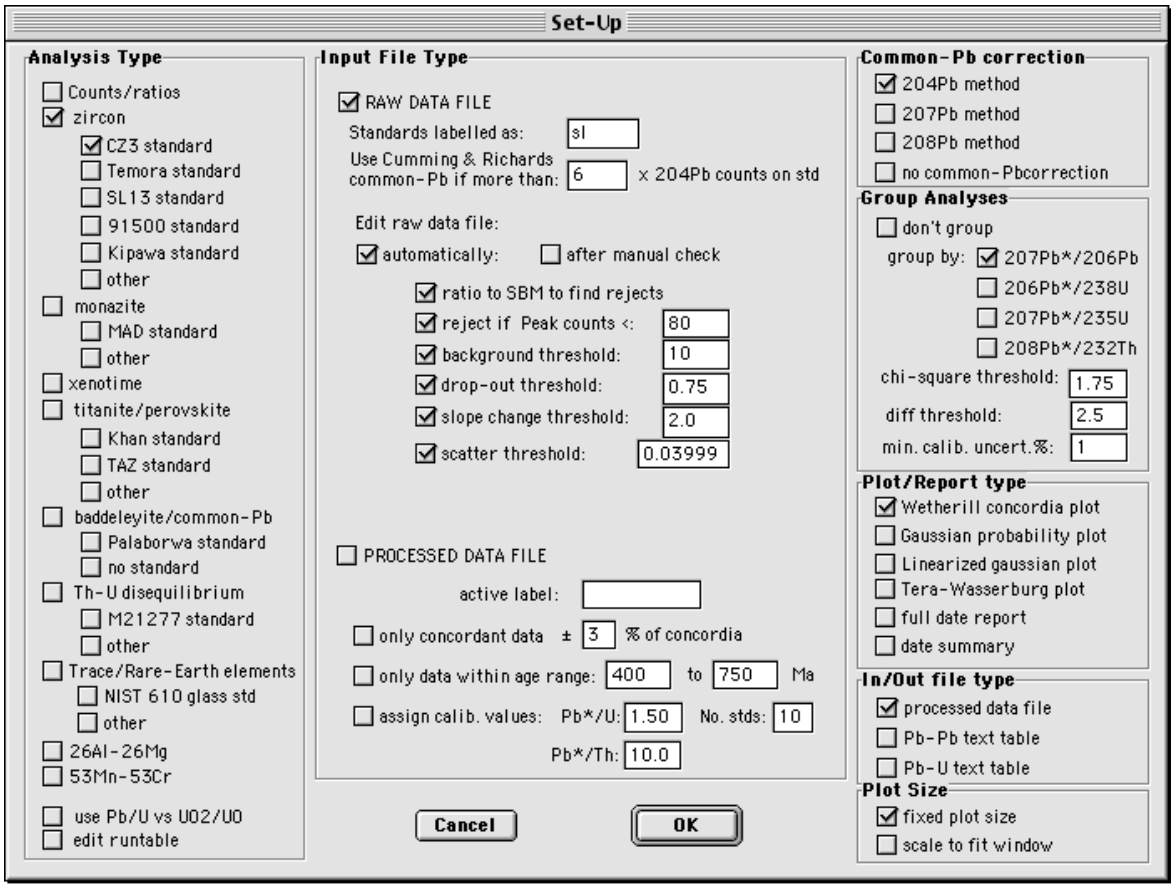

Fig. 3.1. The Set-up dialog (low screen resolution version). Default checkboxes are checked.

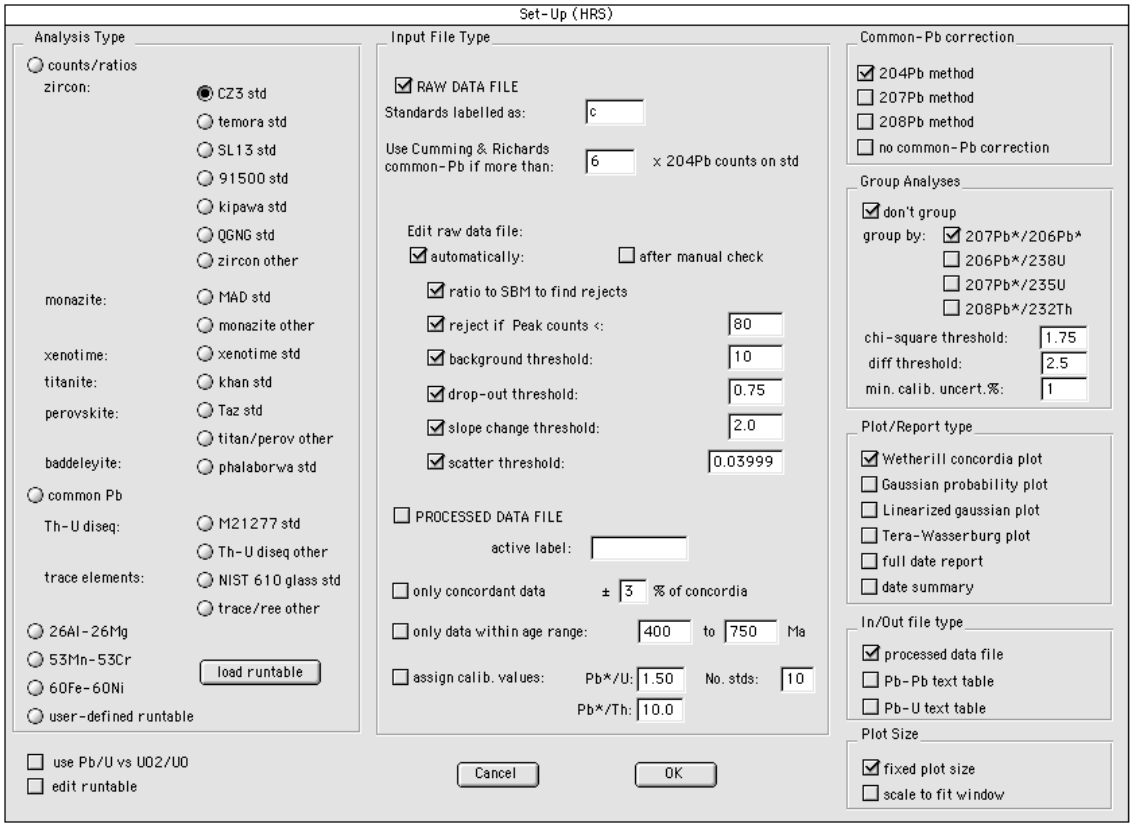

Fig. 3.2. The Set-up dialog (high screen resolution version). Default checkboxes are checked.

3.1 Input (ion-microprobe output) files

An ion-microprobe analysis commonly consists of a matrix of integers, corresponding to the number of secondary ion counts measured over a specified integration time, acquired during one or more passes through the mass spectrum of interest. For example, SIMS U-Pb analysis of a zircon typically involves a series (commonly four to ten sets) of measurements of the abundance of the species $^{90}Zr_2{}^{16}O^+$, $^{204}Pb^+$, background (for example, at mass station 204.1), $^{206}Pb^+$, $^{207}Pb^+$, $^{208}Pb^+$, $^{238}U^+$, $^{248}Th^+$, $^{238}U^{16}O^+$ and possibly also $^{238}U^{16}O_2^+$. The count rate measured at each mass station (after subtraction of the background count rate) is proportional to the secondary ion intensity of each species, determined using an ion counter or faraday cup. Counts may be taken following stepping and adjustment of the mass analyzer to center the ion species of interest on the detector. The count rate measured for each secondary species will usually change systematically during the course of each analysis, as the equilibrium between the electric charge acquired by the sample from the addition of charged primary ions, that lost by the ejection of charged secondary ions, and of electrons lost from the sample via conductive surface, changes.

CONCH has been specifically adapted to read tab-delimited text data files (.op and .sq) such as those output by the Sensitive High-Resolution Ion MicroProbe (SHRIMP; examples of these input formats are given in Appendix 2). The code could be adapted to process single-collector ion-microprobe data files in other formats. Analyses obtained on both standards and unknowns during an entire analysis (typically 24 hr duration) session are typically stored within one or more separate files. Strings within SHRIMP raw data output files are delineated by either a tab or carriage-return (CR) character, whereas analyses are delineated by two CR's. The first line of each analysis consists of a string containing the analysis name, which is entered into the ion-microprobe acquisition software prior to the analysis. A CONCH input file, consisting of the analyses of unknowns along with the standard analyses appropriate for these unknowns, may be readily created using any text editor.

CONCH distinguishes between standard analyses and analyses of unknowns from different samples in the input file by the matching of part of the analysis label string with User-specified standard and sample label strings specified in the Set-up and Standards dialogs. Standard and sample labeling in the CONCH input file should therefore be consistent. The User may specify a label string to identify

standard analyses in the Set-up dialog; separate labels for concentration and Pb/U standards may be defined using the Run-table dialog. CONCH will by default also recognize strings that commence with characters denoting commonly used names for standard minerals (SL, Sl, sl, cz, Cz, Mad, Taz, etc.) as indicating that the analysis is of a standard, and treat the analysis accordingly.

Currently there are two commonly used formats of data file output by the SHRIMP Acquisition program. SHRIMP Acquisition output files with file names ending with ".op" are in the old format, whereas those with file names ending with ".sq" contain additional information about the mass species in each analysis. The mass species labels in the file are those entered into the Acquisition run-table prior to SHRIMP analysis. If an ".sq" file is input, CONCH will check the mass species label strings in the ".sq" file against those specified in the CONCH run-table. If inconsistencies are identified, CONCH can use the mass species information in the file to construct a new run-table using the information read from the ".sq" file, for data processing. This new run-table will be displayed for User approval or editing. Because of the additional information contained in ".sq" files, use of this file type for data processing is preferred to that of the ".op" file type, provided that the mass species label strings used are easily interpretable. To facilitate such checking, the mass species strings used in the SHRIMP Acquisition program run-table should follow a consistent format. For ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr, ^{60}Fe-^{60}Ni analyses, mass species labels the following format (i.e. first two characters of string correspond to the chemical element, with the following characters corresponding to the mass number of the isotope) has been adopted by CONCH: "Backgnd", "Mg24", "Mg25", "Mg26", "Al26", Cr50", "Cr52", "Cr53","Cr54", "Mn55", "Fe58", "Ni58", "Ni60", "Ni61", "Ni62" and "Ni64". Ensure that all analyses in the input file have the same number of mass species as that specified in the Run-table dialog.

3.2 CONCH processed data output files

Following editing of the counts, CONCH directs processed data to its Report Sheet. However, to allow ion-microprobe data obtained on the same sample during different analysis sessions to be combined, grouped and plotted, processed data output by CONCH may also be written to files in a form that can also be read, combined with new data and further reprocessed by CONCH. Exceptions to this are the processed data output files generated by the Counts/Ratios, ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr, ^{60}Fe-^{60}Ni and REE/trace element analysis types, which cannot be input into CONCH for reprocessing. CONCH-processed data files in four different output formats may be input directly into CONCH. "Processed Data" output files are tab-delimited text files containing the processed data for each unknown in each 94-entry line (or, in the case of "Standards Calibration" output files, 102-entry line), terminated by a carriage return, in the order that they were read from the ion-microprobe (raw data) input file. CONCH will, as a (User-editable) default action, concatenate ".data" to the input (ion-microprobe raw data) file name to name the processed data output file. In addition to its use in determining calibration curves and sensitivity factors, each standard analysis is also processed as an unknown, using calibration values and uncertainties determined from the pooling of all session standards following editing by the User.

Examples of other (simpler) output file types generated by CONCH are provided (in the "examples" folder) with CONCH and described in Appendix 1. The ".PbPbtable" and ".PbUtable" formats output by CONCH may be read by CONCH for reprocessing and plotting, by checking the "Processed Data File" checkbox and selecting the appropriate file format using the "In/Out file type" check-boxes in the Set-up dialog. The "PbPbtable" input file provides a convenient way for processed U–Pb geochronology analytical data generated by means other than CONCH to be entered into CONCH for processing and plotting. The simplest way to achieve this is to open the ".PbPbtable" example file provided using Excel, replace the sample name label, ^{207}Pb*/^{206}Pb*, ±1σ uncertainty, ^{206}Pb*/^{238}U, ±1σ uncertainty, ^{207}Pb*/^{235}U, ±1σ uncertainty column entries with those to be processed and plotted, and use Excel's "Save As" to save a copy of the file as "*Text Only*". As these columns contain the only data that CONCH reads from this file type, the new file may then be input into CONCH for grouping and plotting. Excel may add strings of hidden characters to the ends of files it saves, rendering a file unreadable by CONCH, so it is recommended that, after a file has been opened and saved as "*Text Only*" by Excel, the file be reopened using a Text Editor and any extra characters that may have been added at the end of the file be deleted.

Table 3.1. List of checkbox controls within the control group specifying the Analysis Type in the Set-up dialog, with a description of their functions.

Control Label	Control Function
Counts/Ratios	Sets the analysis type and data processing to that for generalized count rates/ratios
Zircon (default)	Specifies that the analysis type and data processing is for the mineral zircon
CZ3 standard (default)	Sets data processing appropriate for the mineral zircon and standard parameters to those of the CZ3 zircon standard
Temora standard	Specifies that the analysis type and data processing is for the mineral zircon and sets standard parameters to those of the Temora zircon standard
QGNG standard	Specifies that the analysis type and data processing is for the mineral zircon and sets standard parameters to those of the QGNG zircon standard
Zircon: other	Specifies that the analysis type and data processing is for the mineral zircon and displays the Run-table dialog with standards parameter fields set to last-entered values, so that User can view and edit standard parameters
monazite	Specifies that the analysis type and data processing is for the mineral monazite
MAD standard	Specifies that the analysis type and data processing is for the mineral monazite and standard parameters to those of the MAD monazite standard
monazite: other	Specifies that the analysis type and data processing is for the mineral monazite and displays the Run-table dialog with standards parameter fields set to last-entered values, so that User can view and edit standard parameters
xenotime	Specifies that the analysis type and data processing is for the mineral xenotime
titanite/perovskite	Specifies that the analysis type and data processing is for the minerals titanite or perovskite
Khan standard	Specifies that the analysis type and data processing is for the mineral titanite and standard parameters to those of the Khan titanite standard
TAZ standard	Specifies that the analysis type and data processing is for the mineral perovskite or titanite and standard parameters to those of the TAZ perovskite standard
titanite/perovskite: other	Specifies that the analysis type and data processing is for the minerals perovskite or titanite and displays the Run-table dialog with standards parameter fields set to last-entered values, so that User can view and edit standard parameters
Baddeleyite/ common Pb	Specifies that the analysis type and data processing is for the mineral baddeleyite or for common-Pb compositions (e.g. galena, feldspar); Pb isotopes only, or Pb isotopes plus other species (e.g. Zr2O 196)
Phalaborwa standard	Specifies that the analysis type and data processing is for the mineral baddeleyite and standard parameters to those of the Phalaborwa baddeleyite standard
No standard	Specifies that the analysis type and data processing is for Common-Pb compositions (e.g. galena, feldspar); Pb isotopes only, or Pb isotopes plus other species (e.g. Zr2O 196)
Th-U disequilibrium	Specifies that the analysis type and data processing is for Th-U Disequilibrium
M21277 standard	Sets the analysis type and data processing is for Th-U Disequilibrium and standard parameters to those of the M21277 Th-U standard
Th-U disequilibrium: other	Specifies that the analysis type and data processing is for the Th-U Disequilibrium and displays the Run-table dialog with standards parameter fields set to last-entered values, so that User can view/edit standard parameters
Trace/Rare-earth elements:	Specifies that the analysis type and data processing is for trace/rare earth element concentration determinations
NIST 610 glass standard:	Specifies that the analysis type and data processing is for trace/rare earth element concentration determinations and the standard parameters to those of NIST 610 glass
Trace/Rare-earth elements: other:	Specifies that the analysis type and data processing is for trace/rare earth element concentration determination and displays Run-table dialog with standards parameter fields set to last-entered values, so that User can view/edit standard parameters
^{26}Al-^{26}Mg	Specifies that the analysis type and data processing is for ^{26}Al-^{26}Mg and displays the Run-table dialog with default ^{26}Al-^{26}Mg masses and with fractionation and normalization parameter fields set to default values (Mg fractionation corrected using ^{25}Mg/^{24}Mg = 0.12663, normalized assuming terrestrial ^{26}Mg/^{24}Mg = 0.13943) for Mg analysis, so that User can view/edit these parameters
^{53}Mn-^{53}Cr	Specifies that the analysis type and data processing is for ^{53}Mn-^{53}Cr and displays the Run-table dialog with default Mn-Cr masses and with fractionation and normalization parameter fields set to default values (Cr fractionation-corrected using ^{50}Cr/^{52}Cr = 0.051859, normalized assuming terrestrial ^{53}Cr/^{52}Cr = 0.1134507) for Cr analysis, so that User can view/edit these parameters
^{60}Fe-^{60}Ni	Specifies that the analysis type and data processing is for ^{60}Fe-^{60}Ni and displays the Run-table dialog with default Fe-Ni masses and with fractionation and normalization parameter fields set to default values (Ni fractionation-corrected using ^{62}Ni/^{64}Ni = 7.2734037, normalized assuming terrestrial ^{60}Ni/^{62}Ni = 3.9619227) for Ni analysis, so that User can view/edit these parameters
Load runtable	Reads runtable information from a text file and displays the contents in the Run-table dialog (see Appendix 2 for example format of the runtable file)
Use Pb/U vs UO2/UO	Sets the calibration method from the default (^{206}Pb/^{238}U -^{238}U^{16}O/^{238}U) to ^{206}Pb/^{238}U - ^{238}U^{16}O$_2$/^{238}U^{16}O
Edit runtable	Opens the Run-table dialog, showing the default, last-saved (if an "Other" standard mineral checkbox has been selected) or User-selected entries, for viewing and editing by the User

Table 3.2. List of controls in the control group Input File: Raw Data File input type in the Set-up dialog, with a description of their functions.

Control label	Control type	Function
RAW DATA FILE	Checkbox (default)	Sets the input file type to SHRIMP output (raw data) file
Standards labeled as:	Editbox	When the characters specified in the editbox match (case-sensitive) those of the same number of characters in the analysis label in the SHRIMP output (raw data) file, identifies the analysis as that of a standard mineral
Use Cumming & Richards common-Pb if more than:	Editbox (default value = 6)	If the sum of the ^{204}Pb counts measured during an analysis on an unknown are less than the value entered into the editbox times the average ^{204}Pb counts measured on standard analyses obtained during the analysis session, then the default common-Pb composition given in the Run-table dialog will be used. If the sum of the ^{204}Pb counts measured during analysis of an unknown is greater than the value entered into the editbox times the average ^{204}Pb counts measured on standard analyses obtained during the analysis session, then the common-Pb composition will be calculated using the method described by Cumming and Richards (1975). Entering a value ≤1 in this textbox forces use of Cumming and Richards (1975) common Pb for all unknowns read from the input file. By entry of a large number in this textbox, the common Pb correction to unknowns will made using the default Pb isotopic composition specified in the Run-table dialog.
Automatically:	Checkbox (default)	Automatically identifies outliers in the SHRIMP output (raw data) file using the parameters specified in the EDIT RAW DATA FILE editboxes
After manual check:	Checkbox	Plots up counts for each analysis within the SHRIMP output (raw data) file (starting with the first analysis within the file) within plot boxes so that User may identify outliers manually
Ratio to SBM to find rejects	Checkbox (default)	Ratios counts for each analysis read from the SHRIMP output (raw data) file (starting with the first analysis within the file) to those measured synchronously on the Secondary Beam Monitor in order to identify outliers. If any outliers are identified, all counts obtained for that species during the analysis will be plotted within a plot box for assessment by User
Reject if Peak counts <:	Checkbox (default)	Enables Reject Peak counts test if Automatic identification of outliers is specified
Reject if Peak counts <:	Editbox (default value = 80)	Ratios counts for each analysis read from the SHRIMP output (raw data) file (in the same order that analyses are read from the file) to those measured synchronously on the Secondary Beam Monitor in order to identify outliers. If any outliers are identified, all counts for that species obtained during the analysis will be plotted within a plot box for assessment by the User
Background threshold:	Checkbox (default)	Enables Background threshold counts test if Automatic identification of outliers is specified
Background threshold:	Editbox (default value = 10)	Monitors background counts for each analysis read from the SHRIMP output (raw data) file (in the same order that analyses are read from the file) in order to identify counts higher than value specified in the editbox. If any background counts higher than value specified in the editbox are identified, all background counts obtained for the analysis will be plotted within a plot box for assessment by the User
Drop-out threshold:	Checkbox (default)	Enables Background threshold counts test if Automatic identification of outliers is specified
Drop-out threshold:	Editbox (default value = 0.75)	Monitors counts for each scan read from the SHRIMP output (raw data) file in order to identify any scan whose value times that specified in the editbox is higher or lower than the average value of all the other counts. If any scan whose value times that specified in the editbox is higher or lower than the average value of all the other counts are identified, all counts obtained for the species during the analysis will be plotted within a plot box for confirmation by the User
Slope change threshold:	Checkbox (default)	Enables Slope Change test if Automatic identification of outliers is specified
Slope change threshold:	Editbox	Monitors regression slope of counts for each scan read from the SHRIMP output (raw data) file in order to identify any scan that, when excluded from the regression analysis, causes a change in slope value that is greater than that specified in the editbox. If a scan is identified that, when excluded from the regression analysis, causes a change in slope value that is greater than that specified in the editbox, all counts obtained for the species during the analysis will be plotted within a plot box for confirmation as an outlier by the User
Scatter threshold:	Checkbox (default)	Enables Scatter threshold counts test if Automatic identification of outliers is specified
Scatter threshold:	Editbox (default value = 0.03999)	Monitors a parameter proportional to the degree of scatter (comparable to MSWD) of counts about a linear regression line for each scan read from the SHRIMP output (raw data) file in order to identify any scan that, when excluded from the regression scatter analysis, causes a change in the scatter value that is greater than that specified in the editbox. If a scan is identified that, when excluded from the regression analysis, causes a change in scatter value that is greater than that specified in the editbox, all counts obtained for the species during the analysis will be plotted within a plot box for confirmation as an outlier by the User

The "Processed Data" output file type is the file type generated from the Zircon, Monazite, Xenotime, Titanite/Perovskite, Baddeleyite/Common-Pb and Th-U Disequilibrium analysis types. Formats of the processed data files output by CONCH for these analysis types are similar. When reading CONCH-generated processed data files (i.e. when the "Processed Data" check-box on the Set-up dialog is checked), CONCH refers to the "In/Out File type" check-box settings on the Set-up dialog and not to the "Analysis Type" settings. The format of the "Processed Data" output file type is listed in Appendix 3.

Table 3.3. List of controls specifying the processing of the "Processed Data" output file type in the Set-up dialog and description of their functions.

Control label	Control type	Function
PROCESSED DATA FILE	Checkbox	Sets the input file type to one of the readable CONCH "Processed Data" output file types
Active label:	Editbox	When the characters specified in the editbox match (case-sensitive) those of the same number of characters in the analysis label in the "Processed Data" output file, reads the analysis from the input file for grouping, plotting and/or reporting
Only concordant data +/-	Checkbox	Enable analyses within a "Processed Data" output file to be tested for their concordance prior to being plotted or reported
Only concordant data +/- % of Concordia	Editbox	Tests the condition that analyses within a "Processed Data" output file are more concordant than the value in the editbox prior to reading these from the file for grouping, plotting and/or reporting
Only data within range:	Checkbox	Enable analyses within a "Processed Data" output file to be tested for their $^{207}Pb/^{206}Pb$ date prior to reading these from the file for grouping, plotting or reporting
Only data within range:	Editbox	Tests the condition that analyses within a "Processed Data" output file have $^{207}Pb/^{206}Pb$ dates greater than the value in the editbox prior to reading these from the file for grouping, plotting and/or reporting
Only data within range: to Ma	Editbox	Tests the condition that analyses within a "Processed Data" output file have $^{207}Pb/^{206}Pb$ dates less than the value in the editbox prior to reading these from the file for grouping, plotting and/or reporting
Assign calib values:	Checkbox	Enables assignment of values to Pb*/U, Th*/U and number of standards from the Set-up dialog prior to reading analyses from the file for grouping, plotting and/or reporting
Assign calib values: Pb*/U:	Editbox	Assigns the value in the editbox to Pb*/U to the analyses read from the file for grouping, plotting and/o reporting
Assign calib values: Pb*/Th:	Editbox	Assigns the value in the editbox to Pb*/Th to the analyses read from the file for grouping, plotting and/or reporting
Assign calib values: No. Stds:	Editbox	Assigns the value in the editbox to number of standards to the analyses read from the file for grouping, plotting and/or reporting

Table 3.4. List of checkbox controls in the Set-up dialog handling the common-Pb correction, with a description of their functions.

Control Label	Control Function
^{204}Pb method (default)	If RAW DATA FILE checkbox is selected, plots and reports on unknowns corrected for common-Pb using the ^{204}Pb correction method. If PROCESSED DATA FILE checkbox is selected, will read from the "Processed Data" output file, plot and report on unknowns corrected for common-Pb using the ^{204}Pb correction method (Compston et al., 1984)
^{207}Pb method	If RAW DATA FILE checkbox is selected, plots and reports on unknowns corrected for common-Pb using the ^{207}Pb correction method. If PROCESSED DATA FILE checkbox is selected, will read from the "Processed Data" output file, plot and report on unknowns corrected for common-Pb using the ^{207}Pb correction method (Compston et al., 1984)
^{208}Pb method	If RAW DATA FILE checkbox is selected, plots and reports on unknowns data corrected for common-Pb using the ^{208}Pb correction method. If PROCESSED DATA FILE checkbox is selected, will read from the "Processed Data" output file, plot and report on unknowns data corrected for common-Pb using the ^{208}Pb correction method (Compston et al., 1984)
No Common-Pb correction	If RAW DATA FILE checkbox is selected, plots and reports on unknowns data processed without any correction for common-Pb. If PROCESSED DATA FILE checkbox is selected, will read from the "Processed Data" output file, plot and report on unknowns data uncorrected for common-Pb

Table 3.5. List of controls specifying the automatic assignment of analyses to age groups in the Set-up dialog and description of their functions.

Control label	Control type	Function
Don't group	Checkbox	Disables automatic grouping of analyses according to their age
Group by $^{207}Pb/^{206}Pb$:	Checkbox (default)	Enables automatic grouping of analyses according to their $^{207}Pb/^{206}Pb$ age
Group by $^{206}Pb/238U$:	Checkbox	Enables automatic grouping of analyses according to their$^{206}Pb/^{238}U$ age
Group by $^{207}Pb/235U$:	Checkbox	Enables automatic grouping of analyses according to their$^{207}Pb/^{235}U$ age
Group by $^{208}Pb/232Th$:	Checkbox	Enables automatic grouping of analyses according to their $^{208}Pb/^{232}Th$ age
Chi-square threshold:	Editbox	Sets maximum value for chi-square parameter used in determining age groups automatically
Diff threshold:	Editbox	Sets maximum value for diff parameter calculated for each analysis and used to determine whether each is a member of an age group

Table 3.6. List of controls specifying the input/output file, plot and report type, plot size and program control in the Set-up dialog, with description of their functions.

Control Group	Control label	Control type	Function
In/Out file type:	Min. calib. Uncert. %:	Editbox	Sets the minimum Pb/U calibration uncertainty (1σ%); a calculated calibration uncertainty less than the value in the editbox will be assigned this value in Report
In/Out file type:	Processed data file	Checkbox (default)	Sets the CONCH output data file type to the "Processed Data" output file type. If the Input file type is set to Processed Data File, sets the input data file type to "Processed Data" output file type.
In/Out file type:	Pb-Pb text table	Checkbox	Sets the CONCH output data file type to Pb-Pb text table data type. If the Input file type is set to Processed Data File, sets the input data file type to Pb-Pb text table data type.
In/Out file type:	Pb/U text table	Checkbox	Sets the CONCH output data file type to Pb-U text table data type. If the Input file type is set to Processed Data File, sets the CONCH input data file type to Pb-U text table data type.
Plot/report type:	Wetherill Concordia plot	Checkbox (default)	Sets the initial plot to display data to the Wetherill Concordia diagram. Other plots can be selected using the buttons on the Wetherill Concordia plot window
Plot/report type:	Linearized Gaussian plot	Checkbox	Sets the initial plot to display data to the Linearized Gaussian diagram. Other plots can be selected using the buttons on the Linearized Gaussian plot window
Plot/report type:	Gaussian probability plot	Checkbox	Sets the initial diagram to display data to the Gaussian-summation probability density diagram. Other diagrams can be selected using the buttons on the Gaussian probability diagram window
Plot/report type:	Tera-Wasserburg plot	Checkbox	Sets the initial diagram to display data to the Tera-Wasserburg diagram. Other diagrams can be selected using the buttons on the Tera-Wasserburg diagram window
Plot/report type:	Full Date Report	Checkbox	Sets the initial task after reading/processing data to preparing the Date Report. Wetherill and other diagrams can be selected using the Plot button on the Report window
Plot/report type:	Date Summary	Checkbox	Sets the initial task after reading/processing data to preparing a Date Summary. The Wetherill and other diagrams can be selected using the Plot button on the Date Summary window
Plot Size:	Fixed plot size	Checkbox	Sets the diagram size to a constant size. The initial x-axis and y-axis length parameters are read from editboxes in the Plot Options dialog
Plot Size:	Scale to fit window	Checkbox	Sets the diagram size to a proportion of the display window size. The initial x-axis and y-axis length parameters are read from editboxes in the Plot Options dialog
Set-up Dialog control:	Cancel	Button	Cancels (terminates the running of) CONCH and returns control to Excel
Set-up Dialog control:	OK	Button (default)	Checks Set-up parameters and proceeds to read the input file of the type specified selected in the dialog

Throughout this contribution, an asterisk is used to indicate that the Pb abundance has been corrected for the common-Pb component and is the radiogenic component only (e.g. radiogenic component of ^{206}Pb is denoted by ^{206}Pb*).

A "Standards Calibration" output file format, selected using the "Calibration File" button in the Standards dialog, enables standards data from each session to be appended to a preexisting standards data file, for the long-term monitoring of ion-microprobe performance and data quality and of different calibration options. The Standards Calibration output includes additional calibration parameters obtained during the analysis of mineral standards. These may be accumulated within a single "Calibration" file, enabling a long-term record of standard analyses to be acquired. Standard analyses within the Calibration File, uncorrected for common Pb or corrected using either the ^{204}Pb, ^{207}Pb or ^{208}Pb correction methods, may be directly read from the file by CONCH, for grouping, plotting and reporting. The format of the "Calibration File" output file type is listed in Appendix 3.

In addition to the "Processed Data" output file and "Standards Calibration" output file formats described above, CONCH can also generate, and read, files containing ^{204}Pb-, ^{207}Pb- and ^{208}Pb-corrected data in a "table" text format ready for publication. The Counts/Ratios, ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr, ^{60}Fe-^{60}Ni and REE/trace element analysis types generate output files with a much-simplified format.

When opening and reading a data file, CONCH firstly checks aspects of the input data for consistency; processing will cease whenever CONCH encounters ambiguities. This is to minimize the unintended incorporation of incomplete analyses into the processed data file. If CONCH encounters problems reading an input file, the User should examine the file contents and resolve all ambiguities. For example, aborting of an analysis will result in a discrepancy between the analysis scan number indicated in the analysis header and the number of scans recorded. Such analyses should either be

deleted, or the analysis scan number indicated in the analysis header changed to reflect the number of scans recorded.

The default "Counts Sheet" must be visible and active whenever "Run" is selected from the CONCH Menu bar.

4. Analysis run-tables

An ion-microprobe analysis commonly consists of a matrix of integers acquired during one or more passes through the mass spectrum of interest. A generalized report giving ratios and their uncertainties can be generated using CONCH's Counts/Ratios analysis type, but for a more sophisticated treatment (correction of each species for background counts, for example), CONCH requires knowledge of the identity of the mass species in the analysis. A shortcoming of acquisition data files generated by the SHRIMP acquisition software is that they do not specify which species have been measured. The CONCH User must therefore provide the species measured and the measurement order in a "run-table" (see Fig. 4.1). CONCH includes a number of commonly used run-tables as defaults for each mineral (and will make a context-informed guess, informing the User of this, when the number of mass stations specified in the CONCH run-table selected by the User doesn't match that in the input file), but it may occasionally be necessary to modify these default run-tables. For most applications, CONCH presently allows up to 16 mass stations to be specified; for the Trace/Rare-earth analysis type, up to 32 mass stations are allowable. The mass-station order may be edited using the Run-table dialog (see Fig. 4.1), accessed via the Set-up dialog. In order for CONCH to use each species measured appropriately (i.e. as a calibration numerator, or to subtract the background counts from the counts obtained for all other species), CONCH interprets a set of strings (e.g. "Zr2O 196", "Pb206", "Backgnd", "UO2 270", "Cup-in", etc.) that correspond to species having a function recognized by the software. A list of controls, their functions and recognized strings in the Run-table dialog is given in Table 4.1. Unrecognized strings entered into the "mass station labels" editboxes and strings used inappropriately (use of the wrong species as a calibration numerator or denominator, or an attempt to generate a diagram requiring a species not included in the run-table) are trapped and brought to the attention of the User.

CONCH can also read run-table information stored within a text file. Several example run-table files are provided with CONCH in the Examples folder (see Appendix 2 for file format examples). The example run-table files may be modified using any text editor. CONCH uses the Analysis Type (Zircon, Monazite etc.) specified in the Set-up dialog to check the contents of the run-table file, so ensure that the correct Analysis Type is specified before loading a run-table from a file.

CONCH allows any number of Background mass stations to be included in a run-table. Edited count rates from stations labeled "Backgnd" in the run-table will be averaged and the average count rate subtracted from the count rates determined for the other mass stations.

All other analysis details (analysis label, number of sets, scans, stations, counts, integration times, analysis times and secondary beam monitor counts) are assigned for each analysis via the input (SHRIMP raw data output) file, with error-checking to notify the User of any values outside the expected range.

For geochronology applications, different Pb/U calibration and concentration standards may be specified using the Run-table dialog. CONCH matches the labels entered into the Calibration Label and Concentration Label text-boxes in the Run-table dialog to those of the analysis labels in the input file.

Matching of analysis label strings is case-sensitive. The entire string entered into the Calibration Label and Concentration Label text-boxes will be compared to that of the same number of characters of the left-hand side of analysis label strings read from the input file. The length l of analysis label strings may be between $1 \leq l \leq 256$.

By default, CONCH recognizes the following strings as commonly-used standard label designators: "Std", "std", "STD", "SL", "Sl", "sL", "sl", "Sl", "CZ", "Cz", "cZ", "cz", "mad", "MAD", "Mad", "Khan", "KHAN", "khan", "Taz", "TAZ", "taz", "M21277", "m21277", "xtc", "Xtc". These strings may be used on the left-hand side of an analysis label to indicate that the analysis is of a standard.

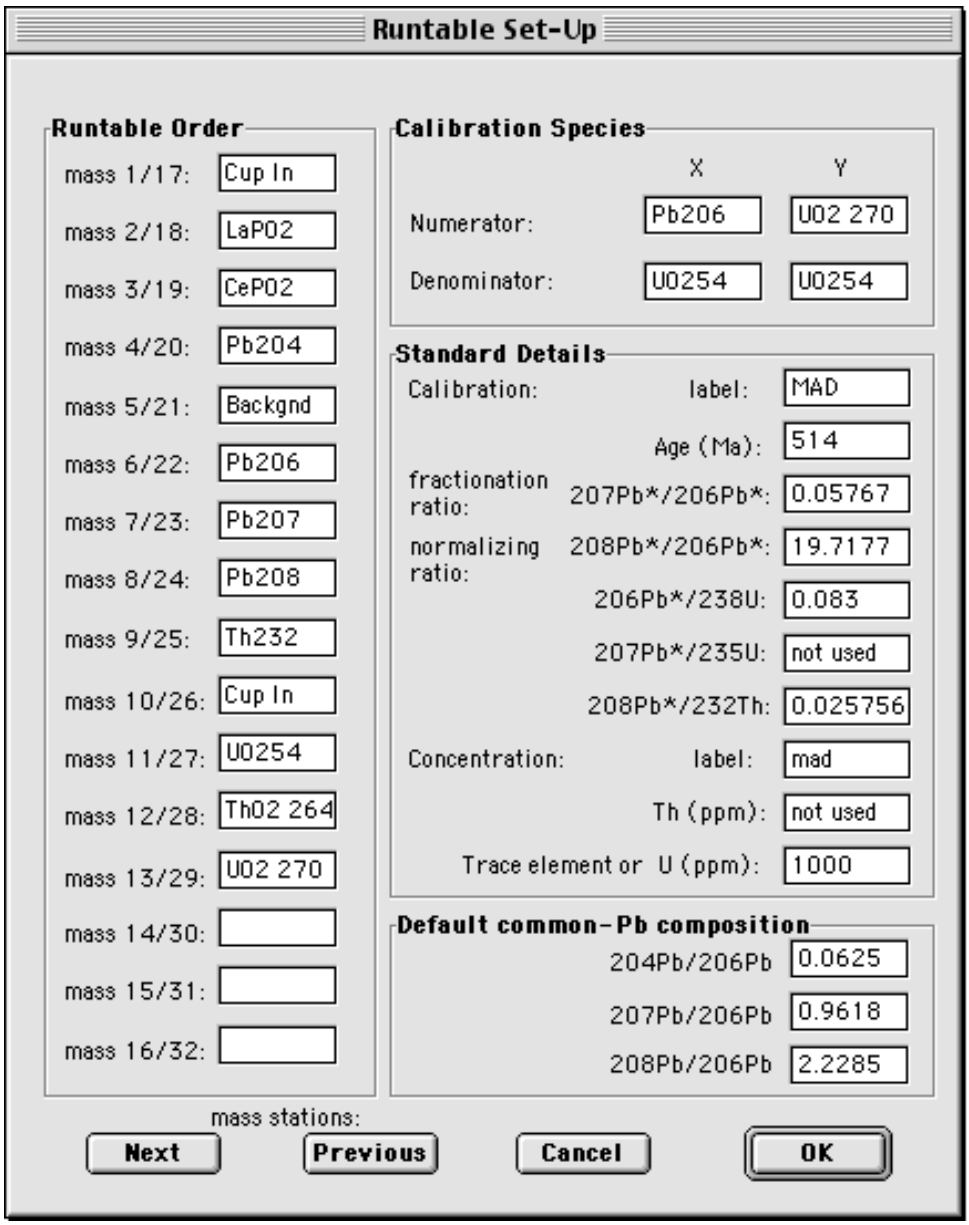

Fig. 4.1. The Run-table dialog.

Table 4.1. List of controls in the Run-table dialog, with a description of their functions.

Control label	Control type	Function
Runtable order: mass 1-16 /17-32:	Editboxes	Displays mass labels of the default or (if "other" is selected in the Analysis Type control group in Set-up) last-used run-table, for editing of order and species analyzed. Valid labels for all analysis types are: Pb204, Backgnd, Pb206, Pb207, Pb208, LaPO2, CePO2, Zr2O196, Th232, U238 ThO248, UO254, ThO2 264, UO2 270, CaTi2O4, Cup In, Au197, Pb208H, ThO246, ThO248, UO250. Any label with"!" as the first character is also valid. If no "Backgnd" mass is specified, User will receive a warning that background corrections will not be made.
Pb/U calibration species: Numerator, X:	Editbox	Displays the mass label of the calibration numerator (for Zircon, Monazite, Zenotime, Perovskite/Titanite and Th-U Disequilibrium analysis types, usually "Pb206") specified in the default or (if "other" is selected in the Analysis Type control group in Set-up) last-used run-table, for editing by User. For ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr, ^{60}Fe-^{60}Ni and Counts/Ratios analysis types, this editbox may be used to specify the numerator of the species to be used for the mass fractionation correction.
Pb/U calibration species: Numerator, Y:	Editbox	Displays the mass label of the calibration numerator (for Zircon, Monazite, Xenotime, Perovskite/Titanite and Th-U Disequilibrium analysis types, usually "UO254" or "UO2 270") specified in the default or (if "other" is selected in the Analysis Type control group in Set-up) last-used run-table, for editing by User.
Pb/U calibration species: Denominator, X:	Editbox	Displays the mass label of the calibration denominator (for Zircon, Monazite, Xenotime, Perovskite/Titanit and Th-U Disequilibrium analysis types, usually "U238" or "UO254") specified in the default or (if "other' is selected in the Analysis Type control group in Set-up) last-used run-table, for editing by User. For ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr, ^{60}Fe-^{60}Ni or Counts/Ratios analysis types, this editbox may specify the denominator of the species to be used for the mass fractionation correction.
Pb/U calibration species: Denominator, Y:	Editbox	Displays the mass label of the calibration denominator (for Zircon, Monazite, Xenotime, Perovskite/Titanit and Th-U Disequilibrium analysis types, usually "U238" or "UO254") specified in the default or (if "other' is selected in the Analysis Type control group in Set-up) last-used run-table, for editing by User. Valid labels are "U238" or "UO254". For ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr, ^{60}Fe-^{60}Ni or Counts/Ratios analysis types, this editbox may specify the species denominator to which all other species will be ratioed.
Standard Data: Calibration: label:	Editbox	When the characters specified in the editbox match (case-sensitive) those of the same number of characters in the analysis label in the Raw data or "Processed Data" output file, identifies the analysis as that of a standard and uses the analysis to determine the Pb*/U calibration line. The Standards label in the Set-up dialog is shown by default.
Standard Data: Calibration: Age (Ma):	Editbox	Displays the Age (in Ma) of the standard specified in the default or (if "other" is selected in the Analysis Type control group in Set-up) last-used run-table, for editing by User
Standard Data: Calibration: 207Pb*/206Pb*:	Editbox	Displays the ^{207}Pb*/^{206}Pb* ratio of the standard specified in the default or (if "other" is selected in the Analysis Type control group in Set-up) last-used run-table, for editing by User. The value in the editbox is used to calculate "hydride" and "excess-204" values. For ^{226}Al-^{26}Mg, ^{53}Mn-^{53}Cr, ^{60}Fe-^{60}Ni analysis types, this editbox may specify the ratio to be used for the mass fractionation correction.
Standard Data: Calibration: 208Pb*/206Pb*	Editbox	Displays the ^{208}Pb*/^{206}Pb* ratio of the standard specified in the default or (if "other" is selected in the Analysis Type control group in Set-up) last-used run-table, for editing by User. The value in the editbox is used to calculate "hydride", "excess-204" and Calc-^{208}Pb/^{206}Pb values. For ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr, ^{60}Fe-^{60}Ni analysis types, this editbox may specify the ratio to be used for normalization of fractionation-corrected ^{26}Mg/^{24}Mg, ^{53}Cr/^{55}Cr or ^{60}Ni/^{62}Ni ratios.
Standard Data: Calibration: 206Pb*/238U:	Editbox	Displays the ^{206}Pb*/^{238}U ratio of the standard specified in the default or (if "other" is selected in the Analysis Type control group in Set-up) last-used run-table, for editing by User. The value in the editbox is used to calculate the^{206}Pb*/^{238}U calibration line.
Standard Data: Calibration: 207Pb*/235U:	Editbox	Displays the ^{207}Pb*/^{235}U ratio of the standard specified in the default or (if "other" is selected in the Analysis Type control group in Set-up) last-used run-table, for editing by User. The value in the editbox is not currently used.
Standard Data: Calibration: 208Pb*/232Th:	Editbox	Displays the radiogenic ^{208}Pb*/^{232}Th ratio of the standard specified in the default or (if "other" is selected in the Analysis Type control group in Set-up) last-used run-table, for editing by User. The value in the editbox is not currently used.
Standard Data: Concentration: label:	Editbox	When the characters specified in the editbox match (case-sensitive) those of the same number of characters in the analysis label in the Raw data input file, identifies the analysis as that of a standard and uses the analysis to determine the U and Th concentrations of unknowns
Standard Data: Concentration: Th (ppm):	Editbox	When the characters specified in the "Standard Data: Concentration: label" editbox match those of the same number of characters in the analysis label in the Raw data input file, identifies the analysis as that of a standard and uses the analysis to determine the Th (and U) concentrations of unknowns
Standard Data: Concentration: U (ppm):	Editbox	When the characters specified in the "Standard Data: Concentration: label" editbox match those of the same number of characters in the analysis label in the Raw data input file, identifies the analysis as that of a standard and uses the analysis to determine the U (and Th) concentrations of unknowns
Dialog control: Next	Button	For Trace/Rare earth elements analysis type, displays the of the mass labels of next 16 masses in the runtable
Dialog control: Previous	Button	For Trace/Rare earth elements analysis type, displays the of the mass labels of previous 16 masses in the runtable
Dialog control: OK	Button (default)	Tests and, if valid, accepts any changes made in the Run-table dialog
Dialog control: Cancel	Button	Cancels any changes made in the Run-table dialog

5. Editing of raw counts data

During measurement using an ion-microprobe, the secondary ion intensity may fluctuate with transient fluctuations in the primary ion intensity, and there may be errors in peak centering of the secondary ion species of interest on the detector. The first step in the processing of ion-microprobe data is the detection of peak-centering problems and aberrant counts on each species.

CONCH enables input data for all species of each analysis to be displayed for manual editing on a set of plots of counts (as checkboxes) for each mass station versus analysis time, on the Counts Sheet (see Fig. 5.1). Counts determined using the Secondary Beam Monitor, measured simultaneously with those of each species, are also plotted. Counting statistics-based "error bars" ($\pm \sqrt{n}$, where n is the number of counts for each measurement) may be added by selecting this option in the Plot Options dialog. A regression line is fitted through the counts obtained for each species. The User may delete any "aberrant" counts by simply clicking on (or "un-checking") their checkboxes. A dropdown control enables the User to display count plots for any new analysis. The "Next Analysis" or "Previous Analysis" menu items in the "CONCH" worksheet menu bar allow the User to step forward and back through the analyses and display their counts sequentially.

Table 5.1 lists the controls on the Counts Sheet and describes their functions.

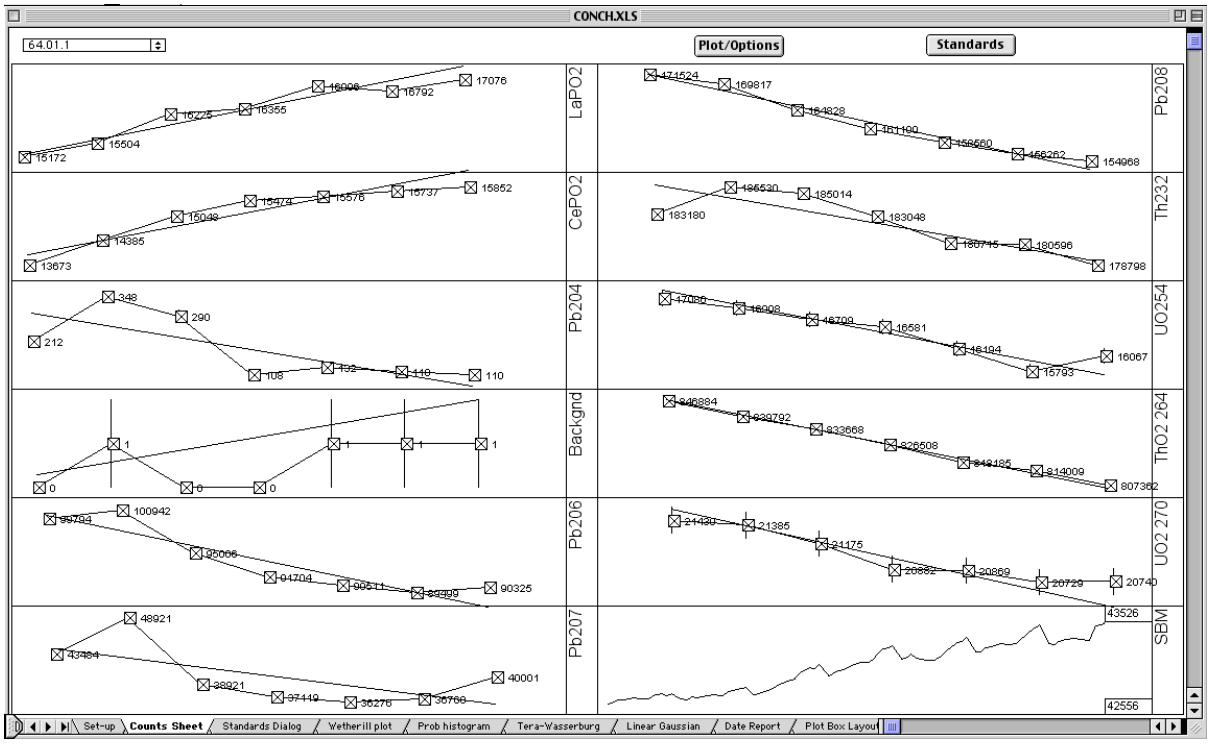

Fig. 5.1. The Counts Sheet.

Due to variations in the screen size and resolution of computers on which CONCH may be run and in the way Visual Basic performs on different platforms, it may be necessary to change aspects of the counts plots, such as the plot box and font sizes. These may be edited via the Plot Options dialog (see Fig. 5.2), which is summoned using the Plot Options button on the Counts Sheet. These need be edited only once when CONCH is first used on a new platform, as the values entered into the Plot Options dialog are read from the dialog edit boxes (even though the dialog is not called by the User) and used as defaults each time "Run CONCH" is selected from the Excel menu-bar. The default plot settings for Macintosh and IBM-compatible platforms may be restored using the "revert to default plot settings" checkbox on the Preferences dialog (see Fig. 2.1).

Table 5.1. List of controls on the Counts Sheet, with description of their functions.

Control Group	Control label	Control type	Function
Raw counts Plot boxes:	mass species	Checkbox (default)	If the Edit Raw Data File manually checkbox in the Set-up dialog is selected, plots the positio of the checkbox for each count within the plot box and includes the count in the calculation of count rates for each species. If the Edit Raw Data File automatically checkbox is selected in the Set-up dialog, displays the plot box for the species containing outliers and un-checks any count considered to be an outlier. If the Counting error-bars checkbox in the Plot Options dialog is selected and the counting statistics-based uncertainty is large enough for the error-ba to extend beyond the checkbox, counting statistic error-bars will be shown.
	Plot Options	Button	Summons the Plot Options dialog, which enables changes to be made to the plot boxes on the Counts sheet and set default parameters for the other diagrams
	Report /Standards	Button	If the analysis type is Counts/Ratios, Al-Mg, Mn-Cr or Trace/Rare earth elements, the "Report" button writes a Generalized Report to the Report Sheet. For all other analysis types, the "Standards" button summons the Standards dialog.

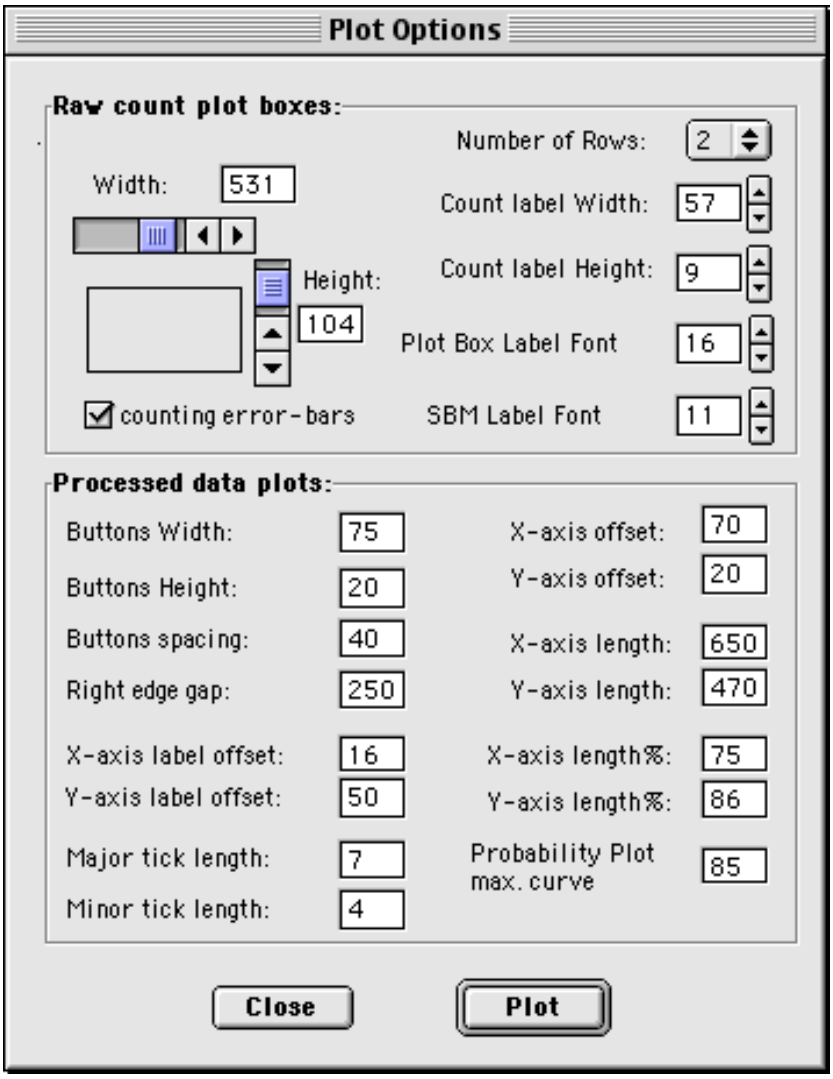

Fig. 5.2. The Plot Options dialog.

Table 5.2. List of controls in the Plot Options dialog, with a description of their functions.

Control label	Control type	Function
Raw count plot box: width	Scrollable Editbox	Adjusts the width of the raw count plot boxes displayed on the Counts Sheet
Raw count plot box: Height	Scrollable Editbox	Adjusts the height of the raw count plot boxes displayed on the Counts Sheet
Raw count plot box: Number of rows	Dropdown box	Changes the number of rows of plot boxes containing the raw counts displayed on the Counts Sheet. Vali options are one or two rows.
Count label Width:	Editbox	Displays and sets the width of the count labels of the checkboxes displayed on the Counts Sheet
Count label Height:	Editbox	Displays and sets the height of the count labels of the checkboxes displayed on the Counts Sheet
Plot Box Label Font Size:	Scrollable Editbox	Displays and sets the font size of the count labels of the checkboxes displayed on the Counts Sheet
SBM Label Font Size:	Scrollable Editbox	Displays and sets the font size of the count labels of the checkboxes displayed in the Secondary Beam Monitor plot box on the Counts Sheet
Counting error-bar	Checkbox	If checked, and the counting statistics-based uncertainty is large enough for the error-bar to extend beyon the checkbox, displays counting statistic ($\pm\sqrt{n}$, where n = number of counts) error-bars on the checkboxes
Buttons width	Editbox	Displays the default width of all buttons on the Counts, Wetherill, Tera-Wasserburg, Linearized Gaussian Gaussian-summation probability density and Report Sheets for editing by the User.
Buttons Height	Editbox	Displays the default height of all buttons on the Counts, Wetherill, Tera-Wasserburg, Linearized Gaussian, Gaussian-summation probability density and Report Sheets for editing by the User
Buttons spacing	Editbox	Displays the default spacing between all buttons on the Counts, Wetherill, Tera-Wasserburg, Linearized Gaussian, Gaussian-summation probability density and Report Sheets for editing by the User
right edge gap	Editbox	Displays the default right edge gap position of the rightmost button on the Counts, Wetherill, Tera-Wasserburg, Linearized Gaussian, Gaussian-summation probability density and Report Sheets for editing by the User
X-axis label offset:	Editbox	Displays the default offset between the *x*-axis label and the axis on the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density Sheets for editing by the User
Y-axis label offset:	Editbox	Displays the default offset between the *y*-axis label and the axis on the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density Sheets for editing by the User
x-axis offset:	Editbox	Displays the default offset between the edge of the sheet and the x-axis on the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density Sheets for editing by the User
Y-axis offset:	Editbox	Displays the default offset between the edge of the sheet and the y-axis on the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density Sheets for editing by the User
x-axis length:	Editbox	Displays the default length of the *x*-axis on the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density Sheets for editing by the User
Y-axis length:	Editbox	Displays the default length of the *y*-axis on the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density Sheets for editing by the User
x-axis length%:	Editbox	Displays the default length of the *x*-axis on the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density sheets as a percentage of the Window width used when the Plot Size: Scale to fit window checkbox in the Set-up dialog is checked, for editing by the User
Y-axis length%:	Editbox	Displays the default length of the *y*-axis on the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density sheets as a percentage of the Window width used when the Plot Size: Scale to fit window checkbox in the Set-up dialog is checked, for editing by the User
Major tick length:	Editbox	Sets the length of the major (labeled) ticks on the *x*-axis and *y*-axis of the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density diagrams
Minor tick length:	Editbox	Sets the length of the minor ticks on the *x*-axis and *y*-axis of the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density diagrams
Probability Plot max. curve height%:	Editbox	Sets the maximum height of the Gaussian-summation probability density curve of all analyses to the percentage of the total plot height specified in the editbox
Plot:	Button (default)	Redraws and plots the plot boxes on the Counts Sheet using the parameters in the Plot Options dialog
Close:	Button	Closes the Plot Options dialog and returns control to the Counts Sheet

In addition to the manual editing of counts for each analysis, CONCH allows automatic identification and display only of scans that include aberrant counts. For automatic identification of outliers, mass-station counts may be ratioed to counts taken on the Secondary Beam Monitor via a checkbox in the Set-up dialog. Count rates for each mass species during an analysis will not necessarily be randomly distributed about a mean value but may change variably as the secondary ion intensity changes. As a consequence, standard statistical techniques based on an assumed distribution function cannot reliably identify count outliers. Software identification of anomalous count values is therefore undertaken using a "neural network" approach, with threshold values for parameters optimised for the detection of the analytical problems commonly encountered and intended to be identified (e.g. peak-centring errors, baseline and peak spikes etc.). Peak-centring errors occur more often during the first measurement of a secondary ion species. One parameter is optimised to identify this sort of outlier by comparing the difference in the slope and scatter of all counts from each mass station, with the slope and scatter for all counts less each one of the count measurements. A second parameter (the "drop-out" parameter on Fig. 3.1) may be optimised to identify other peak-centring errors (anomalously low counts) occurring after the first measurement. A Background counts upper threshold value may also be specified in Set-up to identify spikes at the background (e.g. 204.1) mass station. Data from stations for which anomalous counts are automatically detected will be displayed in diagrams of counts (plotted as checkboxes) versus analysis time, for assessment by the User. Extensive testing has confirmed that this automated data editing can, when the correct threshold settings are used, reliably identify all known instrument-related measurement aberrations, including secondary beam spikes and centring failures (drop-outs). Automated editing thus enables convenient, consistent and efficient identification of aberrant counts. The threshold values of these parameters are displayed and may be edited in the Set-up dialog.

Following identification of outliers using the auto-identify option, only scans that include aberrant counts will be displayed. It is essential that, before accepting or rejecting counts identified automatically as outliers, all of the scans obtained for the entire analysis be examined in order to identify possible causes for the presence of outliers. After noting the names of each of the analyses for which outliers have been identified, scans for each analysis should be displayed, by selecting the analysis name in the pull-down list-item box on the Counts Sheet, and studied. An outlier may be due to transient instability in the primary beam intensity, which may be recognised by instability in the SBM count rates. It may be preferable to delete all counts for the entire scan acquired during such transient instabilities.

Following editing, CONCH determines a count rate for each peak at the mid-time of the analysis by linear regression of the (edited) peak counts. Provided a background mass station has been identified in the Run-table, the background count rate will then be subtracted from each of the mid-time count rates. Ratios of interest and their uncertainties are then calculated using these mid-time count rates. Uncertainties based on counting statistics cannot take into account non-linear change (for example, exponential growth or decay) in the secondary ion intensity during the analysis. However, this systematic "within-analysis" effect should not be confused with uncertainties applicable to an entire analysis; augmentation or reduction of uncertainties, due (for example) to the success of exponential or spline curve fitting of the change in secondary ion intensity during the course of the analysis, may introduce systematic (i.e. non-random) biases into the distribution of ratios obtained for pooled analyses about their weighted mean values. Secondary ion intensity "noise" (arising from instability in the primary ion intensity for example) may increase the scatter of analyses around the weighted mean value beyond that based on counting statistics but because this additional uncertainty is random, it will not significantly bias the mean value of pooled analyses. Additional uncertainty that may be attributable to a high level of random "noise" in the secondary ion intensity is occasionally evident in the slightly elevated chi-square parameter obtained for pooled analyses (see below).

For Counts/Ratios, Trace/Rare-earth elements, ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr and ^{60}Fe-^{60}Ni analysis types, on completion of editing of the raw counts data, a processed data report may be written to the Report Sheet via the "Report" button on the Counts Sheet. To initiate writing of a Report File, the "Save As" dialog may be summoned via the "Report Files" button on the Report Sheet. The Report File should be saved as "text only". For Zircon, Monazite, Xenotime, Titanite/Perovskite, Baddeleyite/Common-Pb and Th-U Disequilibrium analysis types, the Standards dialog (Fig. 7.1) may be summoned via the "Standards" button on the Counts Sheet. Analysis count rates are calculated for each species by linear interpolation

of all measurements made on that species to the mid-time of each analysis, and subtraction of the background counts. These are then used to calculate the ratios of interest.

Because CONCH determines the count rate for each peak at the mid-time of the analysis by linear regression of the (edited) peak counts, subtraction of the observed count rate at the background mass station (calculated by the sum of the counts divided by the total integration time) from that determined by linear regression of the background counts may result in posting of a negative (but near-zero) count rate for the background-corrected background mass station recorded on the Counts/Ratios Report sheet.

6. Correction for the presence of common Pb

In order to calculate $^{206}Pb^*/^{238}U$, $^{207}Pb^*/^{235}U$, $^{208}Pb^*/^{232}Th$ and/or $^{207}Pb^*/^{206}Pb^*$ dates for Zircon, Monazite, Xenotime, Titanite/Perovskite, Baddeleyite/Common-Pb and Th-U Disequilibrium analysis types, measured Pb/U, Pb/Th and Pb isotopic ratios must be corrected for the presence of non-radiogenic (or common) Pb. The contribution from the common-Pb correction to uncertainties in Pb*/U, Pb*/Th and $^{207}Pb^*/^{206}Pb^*$ dates varies as a function of age and can be substantial, particularly for dates younger than c. 1 Ga (see Fig. 6.1). Abundance of the species ^{204}Pb is not affected by radiogenic decay, so the amount of common-Pb present is proportional to the ^{204}Pb abundance detected during the analysis. Therefore, measured Pb isotopic ratios can be corrected for the presence of common Pb using the measured ^{204}Pb count rate. The default method for correcting for the presence of common Pb uses the ^{204}Pb abundance, but CONCH also offers the option of making no corrections, or corrections to Pb*/U and Pb*/Th ratios for the presence of common Pb using the ^{207}Pb- and ^{208}Pb-methods of Compston et al. (1984); these results are written to, and can be read directly and plotted by CONCH from, the "Processed Data" output files. Assumptions required by these methods for the determination of meaningful Pb*/U and Pb*/Th ratios are outlined in Compston et al. (1984).

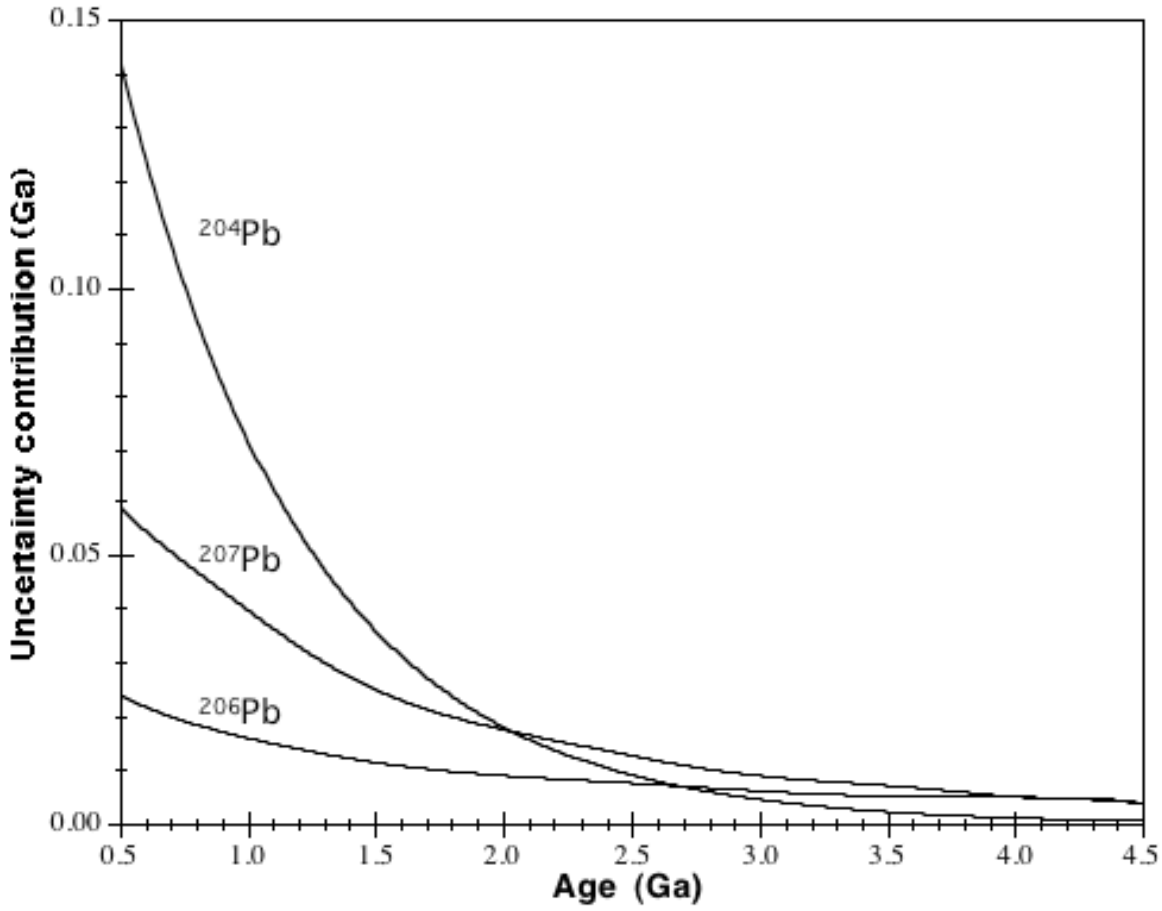

Fig. 6.1. Comparison of the contribution to uncertainties in $^{207}Pb/^{206}Pb$ dates from counting statistics uncertainties associated with measurement of ^{204}Pb, ^{206}Pb and ^{207}Pb abundances. At younger dates, uncertainty in the measurement of ^{204}Pb dominates the age uncertainty, whereas for dates older than 2.5 Ga, uncertainty in ^{206}Pb and ^{207}Pb predominate. The curves assume 750 ppm U. For lower U

concentrations, the ^{204}Pb uncertainty dominates to older dates (i.e. assuming 100 ppm U, ^{204}Pb uncertainty > both ^{206}Pb and ^{207}Pb uncertainties for dates ≤3.0 Ga).

A favorable characteristic of most minerals used for U-Th-Pb geochronology is their incorporation of a large proportion of the available U and Th, yet exclusion of common-Pb from their structure, on their initial crystallization. Most of the common Pb detected during ion-microprobe analysis of high-quality standards may have been added during conductive Au-coating of the surface of the epoxy mount. Due to the long-standing addition of Pb to automotive fuels, common Pb within the modern environment (including that added to the mount surface during Au coating) is dominated by that extracted from only a few major ore deposits. As a consequence, a common-Pb correction assuming an isotopic composition equivalent to that of Broken Hill ore is usually appropriate for these cases. The proportion of "inherent" common Pb derived from within the mineral structure during analyses of unknowns can be estimated by subtraction of the session average ^{204}Pb counts (i.e. that derived from the mount surface) obtained on standard analyses from the measured ^{204}Pb counts. This "inherent" common Pb may have been incorporated into the mineral during, or possibly sometime after, its crystallization. Therefore, an isotopic composition appropriate for the age of the mineral, such as that of the ore Pb growth curve of Cumming and Richards (1975), is appropriate. For analyses of unknowns with ^{204}Pb counts substantially higher than that measured on standards during the analysis session, CONCH incorporates an option for specifying common-Pb compositions calculated using the method of Cumming and Richards (1975). When ^{204}Pb counts (for monazite analyses, corrected for excess ^{204}Pb counts; see below) on unknowns exceed a threshold value specified in Set-up dialog multiplied by the average ^{204}Pb counts measured on the session standards (also corrected for excess ^{204}Pb counts where appropriate), common-Pb corrections are made using Cumming and Richards (1975) model compositions. Entry of a value ≤1 in the textbox in the Set-up dialog ensures use of Cumming and Richards (1975) common Pb for all unknowns read from the input file, whereas entry of a large number in the textbox will ensure that the common Pb correction will made using the isotopic composition specified in the Run-table dialog (the default, but user-editable, composition specified in the Run-table dialog is that of Broken Hill common Pb).

7. Editing of the session standards and determination of Pb/U calibration parameters

7.1 Calculation of Pb/U dates*

Due to differences in their ionization efficiencies during SIMS analysis, the representation of different species in the secondary ion mass spectrum differs from their abundance in the target mineral. Provided that the analysis conditions are constant, the magnitude of this "inter-element fractionation" effect for any specific mineral analyzed during an analysis session is usually approximately constant. Therefore, CONCH corrects for this "inter-element fractionation" effect between Pb and U during any single analysis session, and determines $^{206}Pb^*/^{238}U$ ratios (and Pb/U dates) for unknowns, using the simple relationship:

$$\frac{a_{unk}}{a_{std}} = \frac{A_{unk}}{A_{std}} \qquad (1)$$

where a_{unk} is the observed $^{206}Pb^*/^{238}U$ ratio for the unknown, a_{std} is the observed $^{206}Pb^*/^{238}U$ ratio for the standard, A_{unk} is the fractionation-corrected $^{206}Pb^*/^{238}U$ ratio calculated for the unknown and A_{std} is the "true" $^{206}Pb^*/^{238}U$ for the standard (for the CZ3 zircon standard, $A_{std} = 0.0914$, corresponding to a $^{206}Pb^*/^{238}U$ date of 564 Ma). The $^{206}Pb^*$ abundance used is the radiogenic ^{206}Pb abundance only and has been corrected for the presence of common-Pb; for standard analyses, this correction uses the ^{204}Pb counts determined during each standard analysis and a common-Pb $^{204}Pb/^{206}Pb$ ratio equivalent to that specified in the Run-table dialog (usually that of Broken Hill common Pb ore).

The observed $^{206}Pb^*/^{238}U$ ratio for a standard (a_{std}) is not constant within a session but varies unpredictability with instrument set-up, secondary ion tuning, and operator and sample parameters. Variation in Pb*/U ratios due to inter-element fractionation is correlated with variation in the ratio $^{238}U^{16}O/^{238}U$ (as well as with $^{238}U^{16}O_2/^{238}U$ and $^{238}U^{16}O_2/^{238}U^{16}O$ variation; see below). The relationship between $^{206}Pb^*/^{238}U$ and $^{238}U^{16}O/^{238}U$ variation determined for zircons analyzed using SHRIMP was earlier considered by Compston et al. (1984) to follow a quadratic law. However, a later assessment by Claoué-Long et al. (1995) of U-Pb data from a large number of analytical sessions obtained on the SL-13 zircon standard suggested that the relationship between these parameters may be simplified to a power law of the form:

$$\frac{^{206}Pb^+}{^{238}U^+} = \alpha \times \left(\frac{^{238}U^{16}O^+}{^{238}U^+} \right)^k \qquad (2)$$

The value of α in Equation 2 must be determined from sets of analyses obtained on the standard for each session, or for part of each session if the relationship between these parameters is unstable. On the basis of an investigation of SIMS data obtained for zircon standards during many sessions, Claoué-Long et al. (1995) determined empirically that, for the mineral zircon, $k \sim 2.0$ (see Equation 2) and may be assumed to be constant between analysis sessions (although it is commonly difficult to determine whether the value of k has changed within a single analysis session). As this "power law" relationship results in a linear correlation with slope = k on a $\log_e$-$\log_e$ diagram, it is usually more convenient to calculate and plot $\log_e[Pb^*/^{238}U]$ and $\log_e[^{238}U^{16}O/^{238}U]$, rather than the ratios $Pb^*/^{238}U$ and $^{238}U^{16}O/^{238}U$. CONCH calculates the slope and y-intercept of the $\log_e$ – $\log_e$ calibration correlation, using the (User-specified) calibration species pairs in the Run-table dialog, and displays these in the Standards dialog (Fig. 5). For the processing of unknowns, the User may accept the default slope (i.e. k = 2.0 for zircon) in the "Slope Used" textbox of the Standards dialog, or may insert the calculated regression slope (given in the Regression Slope textbox) if this is preferred. For Zircon, Xenotime and Titanite/Perovskite analysis types, the default calibration ratios are $\log_e[Pb^*/^{238}U]$ and $\log_e[^{238}U^{16}O/^{238}U]$, whereas for the Monazite analysis type, the default ratios are $\log_e[Pb^*/^{238}U^{16}O]$ and $\log_e[^{238}U^{16}O_2/^{238}U^{16}O]$. CONCH fixes the position of the correlation line using weighted mean $\log_e$ values of the calibration ratios specified in the Run-table dialog obtained for the (User-edited) session standards. Using the observed $^{238}U^{16}O/^{238}U$ (or $^{238}U^{16}O_2/^{238}U^{16}O$ or $^{238}U^{16}O_2/^{238}U$, depending on that specified in the Run-table dialog) value for unknowns, the corresponding $^{206}Pb^*/^{238}U$ ratios along the correlation line are determined.

Different methodologies for the determination of monazite U–Pb dates have been previously described by Williams et al. (1996) and Kinny (1997). In order to correct for Pb and U inter-element fractionation during secondary ion mass spectrometric analysis, Williams et al. (1996) assumed a power-law relationship, similar to that used for calculating U–Pb dates for zircons (see above), between the calibration pairs $^{206}Pb^*/^{238}U$ and $^{238}U^{16}O/^{238}U$. Kinny (1997) assumed a simpler linear relationship between the ratios $^{206}Pb^*/^{238}U$ and $^{238}U^{16}O_2/^{238}U^{16}O$. Following a detailed analysis of SHRIMP analytical data obtained on the MAD monazite standard and monazites extracted from a number of samples, a power-law relationship between the ratios $^{206}Pb^*/^{238}U^{16}O$ and $^{238}U^{16}O_2/^{238}U^{16}O$, with a default exponent of 2.0, has been adopted as the default method used by CONCH. However, the calibration species pairs may be readily changed from these default species using the Run-table dialog. The slope and *y*-intercept of the $\log_e - \log_e$ calibration correlation, using the calibration species pairs specified in the Run-table dialog, are displayed in the Standards dialog. For the processing of unknowns, the User may specify the default slope or the calculated regression slope in the Standards dialog (Fig. 7.1), using the "Slope Used" textbox, as was the case of zircon (above).

Inter-element fractionation during SIMS analysis of some minerals may be influenced by high concentrations of some trace elements. For example, relative Pb^+/U^+ fractionation observed for zircon and xenotime samples with high U concentrations (i.e. U > 2000 ppm) is commonly enhanced, resulting in a positive correlation between Pb^+/U^+ and U concentration (Williams and Hergt, 2000; Fletcher et al., 2000) that is unrelated to sample age or discordance. For xenotime analyses, Fletcher et al. (2000) determined a simple relationship between Pb^+/U^+ and U concentration to correct the measured Pb^+/U^+ ratios for this effect. Provided that this option is chosen in the Preferences dialog, CONCH will make these corrections to the measured Pb^+/U^+ ratios obtained for xenotime. The value of the U correction factor (the parameter "f" of Fletcher et al., 2000) is given and may be changed in the Preferences dialog. For the xenotime analysis type, both U-uncorrected and U-corrected Pb^+/U^+ ratios are written to the "Processed Data" output file.

For the determination of Th/U ratios in zircon, CONCH uses the empirically determined relationship between $^{232}Th^+/^{238}U^+$ and $^{238}U^{16}O^+/^{238}U^+$ for zircon described by Williams et al. (1996);

$$\frac{^{232}Th}{^{238}U} = \frac{^{232}Th^{16}O}{^{238}U^{16}O} \times \left[0.03446 \times \left(\frac{^{238}U^{16}O}{^{238}U}\right) + 0.8680\right] \qquad (3)$$

$^{208}Pb^*/^{232}Th$ dates for zircon are calculated using:

$$\frac{^{208}Pb*}{^{232}Th} = \frac{^{206}Pb*}{^{238}U} \times \frac{^{208}Pb*}{^{206}Pb*} \div \frac{^{232}Th}{^{238}U} \qquad (4)$$

CONCH determines $^{208}Pb^*/^{232}Th$ dates for monazite applying the simple relationship given in Equation 1, where a_{unk} is the observed $^{208}Pb^*/^{232}Th$ ratio for the unknown, a_{std} is the "corrected" $^{208}Pb^*/^{232}Th$ ratio for the monazite standard, A_{unk} is the fractionation-corrected $^{208}Pb^*/^{232}Th$ ratio calculated for the unknown and A_{std} is the "true" $^{208}Pb^*/^{232}Th$ ratio for the monazite standard. The "corrected" $^{208}Pb^*/^{232}Th$ ratio for each unknown is calculated using the observed $^{232}Th^{16}O_2/^{232}Th$ ratio and assuming a linear relationship between $^{208}Pb^*/^{232}Th$ and $^{232}Th^{16}O_2/^{232}Th$ values:

$$\frac{^{208}Pb*}{^{232}Th} = \left(\frac{^{208}Pb*}{^{232}Th}\right)_{meas} \times \left(\frac{^{208}Pb*}{^{232}Th}\right)_{std} \div \left\{slope \times \left(\frac{^{232}Th^{16}O_2}{^{232}Th}\right)_{meas} + yintercept\right\} \qquad (5)$$

where *slope* and *y-intercept* is the slope and *y*-intercept of the $^{208}Pb^*/^{232}Th$ and $^{232}Th^{16}O_2/^{232}Th$ calibration line determined from the (User-edited) session standard analyses. The calculated regression slope and *y*-intercept of the calibration line are displayed in textboxes in the Standards dialog. The slope of this relationship ranged from 0.241 to 0.275 and the *y*-intercept from -0.50 to -0.75 during 5 recent monazite analysis sessions. Uncertainties in $^{208}Pb^*/^{232}Th$ ratios for individual monazite analyses do not include uncertainty associated with the determination of the Pb*/Th calibration line, but pooled $^{208}Pb^*/^{232}Th$ dates include an uncertainty estimate based on the reproducibility of the standard $^{208}Pb^*/^{232}Th$ measurements during the analysis session. Uncertainties cited for monazite $^{208}Pb^*/^{232}Th$ dates may be based on the "observed" scatter about the weighted mean $^{208}Pb^*/^{232}Th$ ratio of pooled analyses. A minimum uncertainty for Pb^*/U may be specified in the Set-up dialog; a minimum

uncertainty of 1% (±1σ) is recommended. The decay constants used by CONCH are those recommended by Steiger and Jaeger (1977).

7.2 Editing and assessment of data obtained for standards

For Zircon, Monazite, Xenotime, Titanite/Perovskite and Th–U Disequilibrium analysis types, $\log_e[^{206}Pb^*/^{238}U]$ ratios (corrected for common-Pb using Pb isotopic compositions of Broken Hill common Pb and the measured ^{204}Pb counts), obtained on the standard are plotted in the Standards dialog plot window (see Fig. 6) as checkboxes against $\log_e[^{238}U^{16}O^+/^{238}U^+]$ (or $\log_e[^{238}U^{16}O_2^+/^{238}U^{16}O^+]$; the ratios plotted are the default ratios, or those specified in the Run-table dialog if the "OK" button on this dialog was used). Also shown for comparison in the Standards dialog are an uncertainty-weighted regression line of these parameters for the standards and a line with the default slope (i.e. usually 2.0 for zircon using the calibration pair $\log_e[^{206}Pb^+/^{238}U^+] - \log_e[^{238}U^{16}O^+]$). The number of standards, calibration values and slopes, intercepts, uncertainties and MSWD's for uncertainty-weighted $\log_e[^{206}Pb/^{238}U] - \log_e[^{238}UO/^{238}U]$ (default ratios for zircon; $\log_e$[calibration ratios] plotted are those specified in the Run-table dialog if the "OK" button on this dialog was used) and (for monazite) $^{232}Th/^{238}U - ^{238}U^{16}O/^{238}U$ calibration regression values are also displayed in textboxes in the Standards dialog. A list of controls and their functions in the Standards dialog is provided in Table 7.1.

Because the age of the standard mineral is precisely known and the common-Pb composition detected during analysis of standards can usually be estimated reliably (in the case of many high-quality standards, most of that detected will have been added during Au-coating of the mount surface; see above), the availability of three radiogenic decay systems (^{238}U to $^{206}Pb^*$, ^{235}U to $^{207}Pb^*$ and ^{232}Th to $^{208}Pb^*$) for concordant standards enables calculation of two additional parameters that are useful for monitoring of the consistency and accuracy of Pb*/U and Pb isotopic ratios. The presence of Pb-hydride (PbH^+) in the secondary ion mass spectrum will result in the detection of extra counts at the ^{207}Pb and ^{208}Pb mass stations, due to $^{206}Pb^1H^+$ and $^{207}Pb^1H^+$ respectively, and thus, measurement of elevated $^{207}Pb/^{206}Pb$ and $^{208}Pb/^{206}Pb$ ratios. Problems with the determination of the $^{207}Pb^*/^{206}Pb^*$ ratio, such as that resulting from isobaric interference by $^{206}Pb^1H^+$ at mass $^{207}Pb^+$, may be monitored by comparison of the ^{208}Pb-corrected $^{207}Pb^*/^{206}Pb^*$ ratios obtained for analyses on the standard with the expected value, assuming a common Pb composition equivalent to that of Broken Hill common Pb.

Isobaric interferences at $^{204}Pb^+$ may also monitored for each session, by comparison of the ^{208}Pb-corrected $^{204}Pb/^{206}Pb$ ratios obtained for analyses on the standard with the expected value for this ratio and assuming a known common-Pb isotopic composition. Tungsten (W) wire is commonly used to heat the Au during application of the conductive Au coat to the ion-probe mounts; a correction for isobaric interference at $^{204}Pb^+$, attributable to the presence of $^{186}W^{18}O^+$ on the mount surface, may occasionally be necessary, due to incorrect Au-coating technique. CONCH enables corrections to be made for excess ^{204}Pb counts detected during the analysis of standards; the average excess ^{204}Pb counts determined for standard analyses during the analysis session may be subtracted from the measured ^{204}Pb counts obtained for unknown analyses determined during that session, using the "Excess-204 correction" editbox in the Standards dialog (see Fig. 7.1).

Excess ^{204}Pb (calculated using the ^{208}Pb-corrected ^{206}Pb count rate and the common-Pb $^{204}Pb/^{206}Pb$ ratio given in the Run-table dialog), "hydride" values (based on the ^{208}Pb-corrected $^{207}Pb^*/^{206}Pb^*$ ratio), and ^{204}Pb- and ^{208}Pb-corrected $^{207}Pb^*/^{206}Pb^*$ dates, with uncertainties for these parameters for each standard analysis, plus the calculated session means, are displayed in a scrollable list-box next to the calibration plot. Also provided within the scrollable list-box is a brief "diagnosis" statement indicating the significance of these and other relevant parameters (i.e. number of standard analyses for which the background count rates were higher than the ^{204}Pb count rates) obtained for the analysis session, as an aid to their correct interpretation.

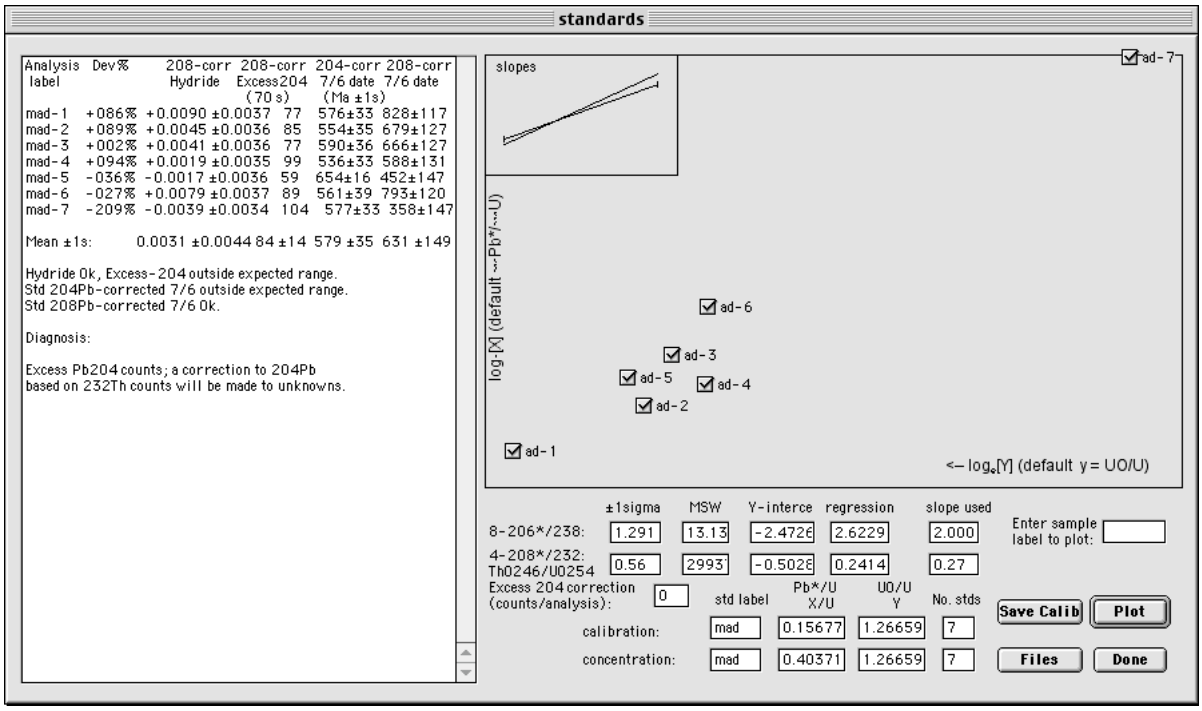

Fig. 7.1. The Standards dialog. To alleviate congestion on the calibration plot, the checkbox labels are truncated and only the last 4 characters are displayed.

A residual interference at ^{204}Pb, attributed to either scattered ions or an unidentified isobar, has been noted in several studies (e.g. Williams et al., 1996; Kinny, 1997; Stern and Sanborn, 1998) for SHRIMP analyses of monazite. Analyses of the MAD monazite standard indicate typical excess-^{204}Pb count rates of 1–2 counts/s. The count rate of this interference was inferred by Kinny (1997) to be proportional to the ^{232}Th count rate. For monazite analyses, CONCH will automatically calculate a correction for this interference at ^{204}Pb, based on the observed relationship between the average values of the excess ^{204}Pb and ^{232}Th counts for the monazite standards during the analysis session (see Kinny, 1997). Provided this option is specified in the Preferences dialog, a correction, in proportion to the ^{232}Th count rate observed for each unknown analysis and the average ^{232}Th count rate observed for the monazite standard during the analysis session, can made to ^{204}Pb counts and ^{204}Pb/^{206}Pb ratios determined for each of the unknowns. It has recently been argued (I.S. Williams, personal communication, 2003) that the isobaric interference at ^{204}Pb may be eliminated by energy filtering of the secondary ion mass spectrum. If no excess-^{204}Pb counts are observed in analyses of the monazite session standards, insignificant or no corrections will be made to analyses of the unknowns. Both uncorrected and corrected ^{204}Pb counts and ^{204}Pb/^{206}Pb ratios are written to the "Processed Data" output files for analyses of monazite.

Standard analyses can be deleted from the calibration line by clicking on their checkboxes within the Standards dialog plot diagram (see Fig. 7.1). Following such editing, recalculated hydride, excess-^{204}Pb, calibration slope and intercept, and calibration uncertainties are displayed in the Standards dialog listbox and editboxes. The default slope, the best estimate of the calibration slope based on replicate high-quality analyses from well-behaved sessions, will be displayed in the "Slope Used" editbox, but (as explained above) the User may insert the session calculated regression slope (or any other preferred value) into the "Slope Used" editbox.

7.3 Determination and treatment of Pb/U calibration uncertainties*

Uncertainties determined by CONCH for individual analyses include those arising from counting statistics and in the corrections for the presence of common Pb (see section 5 above for details). For individual analyses, CONCH also provides uncertainties for Pb*/U ratios that includes those arising from counting statistics and in corrections for common Pb, but augmented by a contribution associated

with the determination of the Pb/U – UO/U calibration curve (i.e. in the constant α in Equation 1 given above) based on the reproducibility of the standard Pb/U measurements.

Uncertainties in Pb*/U ratios for age groups derived from pooled analyses may also include uncertainty in the Pb*/U calibration, *E*, based on the reproducibility of the Pb*/U ratios of standard measurements,

$$E = \frac{C \times \mu_n}{\sqrt{n}} \qquad (6)$$

where C is the calibration uncertainty (σ) based on reproducibility of standard determinations, μ_n is the weighted mean Pb*/U ratio determined for pooled analyses of unknowns and *n* is the number of standard determinations. This uncertainty may be summed in quadrature with the other sources of uncertainty.

The validity of the addition (in quadrature) of a calibration uncertainty based on reproducibility of Pb*/U ratio measurements of standards to Pb*/U ratios obtained for unknowns has recently been the subject of considerable contention (see Compston, 1999, 2001; Black and Jagodzinski, 2003). Disagreement concerns the causes of scatter, observed for the analyses of standards during SHRIMP analysis sessions, that is in excess of that attributable to counting statistics and corrections for common Pb. Compston (1999, 2001) attributed this additional scatter to heterogeneity in Pb/U within the standards that would not be expected to effect analyses of unknowns, whereas Black and Jagodzinski (2003) attributed it to instrumental causes that will effect analyses of both standards and unknowns. Black and Jagodzinski (2003) and Stern and Amelin (2003) presented evidence confirming that the scatter in Pb*/U ratios determined using SHRIMP and the Pb/U – UO/U calibration approach is in excess of that attributable to sample Pb/U heterogeneity. If the excess scatter in Pb*/U (and also in Pb*/UO and Pb*/UO_2) is due to an inherent inadequacy arising from use of the UO/U ratio (and also UO_2/U and UO_2/U) to correct for the large inter-element fractionation between Pb and U during SIMS measurements, as proposed by Stern and Amelin (2003), then such uncertainty should be propagated to corrected Pb*/U ratios determined by this method. However, reproducibility in Pb*/U is also a function of U and Pb count rates, which are dependent on U and Pb abundance in the target mineral, and on common-Pb corrections. As a consequence, reproducibility of the Pb*/U ratio for standards can only approximate that appropriate for unknowns.

For pooled analyses, CONCH calculates an "observed" uncertainty, based on the observed distribution of analyses about the weighted mean value, and an "expected" uncertainty determined by the addition in quadrature of uncertainties for individual analyses determined from counting statistics and the common-Pb correction. In addition, CONCH provides the User with a choice of two other uncertainty levels for fractionation-corrected Pb*/U ratios; those based on "observed" and "expected" uncertainties but with an additional uncertainty, based on reproducibility of the session standards, added to each analysis in quadrature, and those to which an uncertainty, based on reproducibility of the session standards, has been added in quadrature to the pooled "observed" and "expected" uncertainties. Provided that the reproducibility estimated from the Pb*/U ratio for standards is appropriate for unknowns, the pooled "observed" and "expected" uncertainties should be identical. The chi-square parameter (see below) provides a convenient means of assessing whether this is the case.

Chi-square (χ^2) tests whether the observed frequencies in a distribution differ significantly from the frequencies that might be expected according to some assumed hypothesis (Moroney, 1984, p. 249). A chi-square test may be applied to grouped analyses in order to assess the relative effects of analytical sources of uncertainty, such as counting statistics, and geological sources of error, such as that arising from the inclusion of analyses of slightly older xenocryst zircons or zircons that may have lost small amounts of radiogenic Pb. The chi-square parameter compares the uncertainty determined from the observed distribution of individual analyses about the weighted mean value, with the uncertainty determined by addition in quadrature of the uncertainty for individual analyses based on counting statistics, the inter-element (Pb*/U and Pb*/Th) calibration (where appropriate) and the common-Pb correction;

$$\chi^2 = \frac{1}{(n-1)} \times \sum_{i=1}^{n} \frac{(x_i - \mu_n)^2}{\sigma_n^{\,2} + \sigma_i^{\,2}} \qquad (7)$$

where n is the number of pooled x_i values ($^{207}Pb/^{206}Pb$, $^{207}Pb^*/^{206}Pb^*$, $^{206}Pb^*/^{238}U$, $^{207}Pb^*/^{235}U$ or $^{208}Pb^*/^{232}Th$ ratios), μ_n is the weighted mean of all pooled x_i values, σ_n is the uncertainty in μ_n calculated by addition of all weighted individual uncertainties in quadrature, and σ_i is the uncertainty in the ratio x_i. Chi-square values for grouped analyses of less than or equal to unity indicate that scatter about the weighted mean value determined for the grouped analyses can be accounted for by analytical sources of uncertainty alone. A chi-square value significantly greater than unity indicates that analyses are not normally distributed about the weighted mean value and that other (geological) sources of uncertainty are present within the grouped population. In these cases, the 95% confidence uncertainty cited for dates should based on the observed, rather than the expected, scatter about the weighted mean $^{207}Pb/^{206}Pb$ (or Pb*/U) ratio of pooled analyses.

CONCH provides uncertainties for individual analyses in the output files and in the Report dialog at the 1σ level, whereas for pooled analyses, uncertainties are also cited at tσ (where t is Fisher's t), equivalent to 95% confidence.

7.4 Coping with an unstable standard Pb/U calibration*

If the pooled standard results for an analysis session indicate a ^{208}Pb-corrected Pb*/U calibration uncertainty >3.5% and a secular change in Pb*/U is evident in the standard analyses, regrouping into smaller groups may be justified. The simplest approach is to duplicate the input file for each subgroup and delete all analyses that appear before the end of one subgroup and the beginning of the next subgroup. To obtain an adequately constrained calibration line, minimum of 4 standard analyses for each subgroup is recommended.

7.5 Determination of U, Th and Pb concentrations

Because homogeneous mineral standards with both constant Pb/U ratios and constant U concentrations are scarce, CONCH enables determination of Pb/U ratio and U concentration calibration lines using two separate (calibration and concentration) standards, where this is necessary. The concentration standard analysis label and U concentration may be specified in the Run-table dialog.

Uranium concentrations are determined by ratioing the U count rate to that determined for a major, preferably stoichiometric, component of the mineral and using the approach outlined in Equation 1, with a_{unk} equal to the observed $^{238}U/m$ ratio (where m is a known component of the mineral) for the unknown, a_{std} the observed $^{238}U/m$ ratio for the standard (for the CZ3 zircon standard, a U concentration of 550 ppm is assumed), A_{unk} the fractionation-corrected $^{238}U/m$ ratio calculated for the unknown and A_{std} corresponding to the "true" $^{238}U/m$ ratio for the standard. For zircon, concentrations are commonly ratioed to the count rates obtained for the species $^{90}Zr_2{}^{16}O$. Th and Pb concentrations are determined using the Uranium concentration and the Th/U (Equation 3). For xenotime, the near-stoichiometric Y_2O count rates are used, whereas for monazite, there is no suitable near-stoichiometric component available for determining trace-element concentrations. Approximate U and Th concentrations for monazite are calculated using $CePO_2$ count rates and using $^{238}U^{16}O_2/^{238}U^{16}O$ (instead of $^{238}U^{16}O/^{238}U$) and Pb*/U relationships.

7.6 Calibration data compilation and the processing of unknowns

The "Calibration File" button on the Standards dialog provides a means of monitoring the analytical performance of the ion microprobe over the long term, by allowing the edited standards to be appended to a processed standards output file. As outlined earlier, this button enables the standards data displayed in the dialog to be appended to an existing "Calibration" file, for long-term monitoring of data quality. The "Files" button on the Standards dialog allows a "Processed Data" output file to be written to disk. Because analyses of unknowns have not yet been assigned to age groups, the "Age Group" column entry within "Processed Data" output files written using the "Files" button on the Standards dialog is assigned a zero value. If "Age Group" data are required within the file, the "Processed Data" output file should be written using the "Files" button on the Report sheet. Also on the Standards dialog is a "Done" button, for terminating CONCH program execution.

Table 7.1. List of controls in the Standards dialog, with a description of their functions.

Control label	Control type	Function
	Listbox	Lists the standard analysis label, percent deviation (Dev%) from the calibration line with default slope, difference in ^{208}Pb-corrected ^{207}Pb*/^{206}Pb* ratio from the expected ^{207}Pb/^{206}Pb ratio for the standard ("hydride"), calculated uncertainty in the ^{208}Pb-corrected ^{207}Pb/^{206}Pb ratio, excess ^{204}Pb counts (calculated using measured ^{204}Pb, ^{208}Pb-corrected ^{204}Pb*/^{206}Pb* and the expected ^{204}Pb/^{206}Pb ratio for the standard), calculated uncertainty in the excess ^{204}Pb counts, calculated ^{204}Pb-corrected ^{207}Pb/^{206}Pb age and its uncertainty, calculated ^{208}Pb-corrected ^{207}Pb/^{206}Pb age and its uncertainty, Mean values for "hydride", exces ^{204}Pb counts and ^{204}Pb-corrected ^{207}Pb/^{206}Pb age with observed uncertainties, ^{208}Pb-corrected ^{207}Pb/^{206}Pb age with observed uncertainties. If any of these parameters are outside the expected range at the ±1σ uncertainty level, a brief diagnosis of possible causes is given.
8-206*/238, 1sigma%:	Editbox	Displays the ^{206}Pb/^{238}U calibration uncertainty (1σ%) calculated using the standard analyses in the Standard dialog calibration diagram whose checkboxes are checked
8-206*/238, MSWD:	Editbox	Displays the MSWD calculated for points used to determine the ^{206}Pb*/^{238}U calibration line, using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked
8-206*/238, Y-intercept:	Editbox	Displays the ^{206}Pb*/^{238}U calibration regression line *y*-intercept calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked
8-206*/238, regression slope:	Editbox	Displays the ^{206}Pb*/^{238}U calibration regression line slope calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked
8-206*/238, slope used:	Editbox	Displays the ^{206}Pb*/^{238}U calibration default slope. When either of the "Plot" or "Files" buttons on the Standards dialog are selected, the value in this editbox will be read from the dialog and used as the calibration slope for the processing of unknowns analyzed during the session.
4-208*/232, ThO246/UO254, 1sigma%:	Editbox	For the Zircon analysis type, displays the ^{204}Pb-corrected ^{232}Th/*^{208}Pb^{+} vs ^{238}U^{16}O^{+}/^{238}U^{+} calibration uncertainty (1σ%) calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked. For the Monazite analysis type, displays the ^{208}Pb/^{232}Th^{+} vs ^{238}U^{16}O$_2^{+}$/^{238}U^{16}O^{+} calibration uncertainty (1σ%) calculated by regression of the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked
4-208*/232, ThO246/UO254, MSWD:	Editbox	For the Monazite analysis type, displays the MSWD for the ^{204}Pb-corrected ^{208}Pb/^{232}Th^{+} vs ^{238}U^{16}O$_2^{+}$/^{238}U^{16}O^{+} calibration uncertainty (1σ%) calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked
4-208*/232, ThO246/UO254, Y-intercept:	Editbox	For the Monazite analysis type, displays the y-intercept for the ^{204}Pb-corrected ^{232}Th/^{208}Pb^{+} vs ^{238}U^{16}O$_2^{+}$/^{238}U^{16}O^{+} calibration regression line calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked
4-208*/232, ThO246/UO254, regression slope:	Editbox	For the Monazite analysis type, displays the regression slope for the ^{204}Pb-corrected ^{232}Th/^{208}Pb^{+} vs ^{238}U^{16}O$_2^{+}$/^{238}U^{16}O^{+} calibration line calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked
4-208*/232, ThO246/UO254, slope used:	Editbox	For the Monazite analysis type, displays the default slope for the ^{204}Pb-corrected ^{232}Th/^{208}Pb^{+} vs ^{238}U^{16}O$_2^{+}$/^{238}U^{16}O^{+} calibration line. When the Plot button in the Standards dialog is selected, the entry in the default slope editbox is read from the dialog and will be applied for the processing of unknown analyses.
Excess-204 corr:	Editbox	Contains the counts that will be deducted from the measured ^{204}Pb counts obtained for unknown analyses, in order to correct for excess ^{204}Pb counts detected during the analysis of the session standards
Zr/U, La/U, CaTiO2/UO, Au/U:	Editbox	For the Zircon analysis type, displays the mean ^{96}Zr$_2$^{16}O^{+}/^{238}U^{+} calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked. For the Monazite analysis type, displays the mean LaPO$_2$/^{238}U^{+} calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked. For the Perovskite/Titanite analysis type, displays the mean CaTiO$_2^{+}$/^{238}U^{16}O^{+} calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked. If the Th-U Disequilibrium analysis type, displays the mean ^{197}Au^{+}/^{238}U^{+} calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked.
Pb*/U, X:	Editbox	Displays the weighted mean Calibration X ratio (default for zircon is radiogenic ^{206}Pb^{+}/^{238}U^{+}) calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked
UO/U, Y:	Editbox	Displays the weighted mean Calibration Y ratio (default for zircon is ^{238}U^{16}O^{+}/^{238}U^{+}). If "Use Pb/U vs UO2/UO" in the Analysis Type control group of the Set-up dialog is not checked, displays the weighted mean ^{238}U^{16}O^{+}/^{238}U^{+} calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked. If the "Use Pb/U vs UO2/UO" in the Set-up dialog is checked, displays the weighted mean ^{238}U^{16}O$_2^{+}$/^{238}U^{16}O^{+} calculated using the standard analyses in the Standards dialog calibration diagram whose checkboxes are checked.
No. stds:	Editbox	Displays the number of standards in the Standards dialog calibration plot whose checkboxes are checked
Plot diagram:	Check-boxes	If checked, indicates that standard analysis has been used in the calculation of the ^{208}Pb-corrected Pb*/U (and Pb*/Th as appropriate) calibration lines
Enter sample label to plot:	Editbox	Plots or prepares a report that includes all analyses in the input file with analysis labels that match (case-sensitive) those of the same number of characters specified in the editbox
Plot:	Button (default)	Uses the checked standard analyses in the standards dialog calibration diagram to determine the Pb/U (or if appropriate, Pb/Th) calibration line, applies this to the unknowns and displays on the default diagram or prepares a Date Report, according to that specified in the Set-up dialog
Calibration file	Button	Uses the checked standard analyses in the standards dialog calibration diagram to determine the Pb/U (or if appropriate, Pb/Th) calibration line and applies these to all standard analyses, summons the "Save As" dialog and appends processed data obtained for all session standards to a preexisting Calibration File
Files	Button	Using the checked standard analyses in the standards dialog calibration diagram to determine the Pb/U (or if appropriate, Pb/Th) calibration line, specifies that processed data is to be written to a "Processed Data" output file, and summons the "Save As" dialog. Analysis groups within the "Age Group" column in the "Processed Data" output file will be assigned zero.
Done	Button	Returns control to Excel

Once editing of the standards is complete, a string corresponding to the diagnostic part of the sample labels in the input file may be entered into a Sample Label textbox on the Standards dialog, to identify analyses to be graphed or tabulated within the Date Report on the Report Sheet. The "Plot" button will then initiate grouping of analyses of unknowns if this was specified in the Set-up dialog, and preparation of the diagram or report type specified.

8. Assignment of analyses to age groups

Analyses may be automatically assigned to $^{207}Pb/^{206}Pb$ or common-Pb-corrected $^{207}Pb^*/^{206}Pb^*$, $^{206}Pb^*/^{238}U$, $^{207}Pb^*/^{235}U$ or $^{208}Pb^*/^{232}Th$ age-groups (depending on that specified in Set-up) and displayed on Wetherill Concordia (Wetherill, 1956), Tera-Wasserburg Concordia (Tera and Wasserburg, 1974) or Linearized Gaussian diagrams in a group fill color, or on a Gaussian-summation probability density diagram. For the assignment of analyses to age groups, CONCH uses a statistically rigorous algorithm based on the following procedure. Common-Pb uncorrected or radiogenic $^{207}Pb^*/^{206}Pb^*$, $^{206}Pb^*/^{238}U$, $^{207}Pb^*/^{235}U$ or $^{208}Pb^*/^{232}Th$ ratios are weighted according to the inverse square of the individual analytical uncertainty to determine a weighted mean ratio for all pooled analyses obtained for the sample. Analyses are then rejected from the group using two criteria. A chi-square value (see above) is calculated for the grouped analyses. If the chi-square value is greater than a User-editable threshold value specified in Set-up (typically, a chi-square threshold value of 1.75 is used), geological sources of uncertainty are assumed to be present within the group and the analysis whose ratio with assigned uncertainty is most different from the weighted mean value will be excluded from the group. In addition, a measure of the difference (D) between each analysis and the population weighted mean is calculated as follows:

$$D = \frac{x_i - \mu_n}{\sqrt{\sigma_{pop}{}^2 + \sigma_i{}^2}} \qquad (8)$$

where x_i is the analysis ratio, σ_i is the analysis standard deviation, μ_n the population weighted mean and σ_{pop} is the population standard deviation. Any ratio whose calculated D value is greater than a User-editable threshold value (typically, a threshold of ±2.5 is used) from the group weighted mean will also be deleted from the group. The weighted mean value of the remaining analyses is then recalculated. This process is repeated until all remaining analyses are within both parameter thresholds. Analyses that belong with a valid group are then excluded from the pool and the process repeated until all remaining analyses have been grouped. This grouping method is statistically conservative, in that only the minimum number of clearly resolvable dates based on the uncertainty limits assigned to each individual analysis will be identified. Analyses with assigned uncertainties overlapping more than one age group will be assigned to the larger group (i.e. group containing more analyses), as larger groups are usually identified earlier during the grouping procedure. Extensive testing has confirmed that this automated grouping method is robust and generally superior to manual (and potentially subjective) analysis grouping methods. If required, analyses may be manually reassigned between groups on the Report Sheet (see below) and replotted.

9. Plotting of unknowns

U-Pb analyses may initially be plotted on either Wetherill Concordia (Wetherill, 1956; Fig. 9.1), Tera-Wasserburg Concordia (Tera and Wasserburg, 1974; Fig. 9.2), Linearized Gaussian (Fig. 9.3) or Gaussian-summation probability density (Fig. 9.4) diagrams, depending on that specified in the Set-up dialog. Buttons along the base of the plot windows allow the User to readily move between these diagrams and the Report Sheet. Where $^{206}Pb^*/^{238}U$ and/or $^{207}Pb^*/^{235}U$ ratios are unavailable (e.g. common Pb and baddeleyite analyses), $^{207}Pb/^{206}Pb$ or ^{204}Pb-corrected $^{207}Pb^*/^{206}Pb^*$ ratios may be plotted on Linearized Gaussian or Gaussian-summation probability density diagrams. On all of these diagrams, CONCH initially determines the *x*- and *y*-axis ranges, labels and tick intervals, based on the ranges of the data to be plotted. However, the plot position, size and aspect, axis ranges, labeling, tick intervals and other aspects of the plots are User-editable and may be personalized via the "Plot Options" dialog (Fig. 5.2), and via the "Edit" dialogs (Figs. 9.5 and 9.6) summoned by the "Edit" button on each of the plot windows. As an aid to the User, CONCH will add a text string to the Wetherill and Tera-Wasserburg Concordia diagrams listing any analyses that may plot outside the axis ranges selected by the User. Lists of the controls and a description of the control functions in the Plot Options and Preferences dialogs, and on the Wetherill, Tera-Wasserburg, Linearized Gaussian and Gaussian-summation probability density Sheets are given in Tables 9.1 to 9.4.

On the Wetherill Concordia diagram, *x*- and *y*-axis uncertainties are correlated. Therefore, analyses on this diagram are displayed as ±1σ uncertainty polygons that include the 1σ-level uncertainty in each of *x* ($^{206}Pb^*/^{238}U$), *y* ($^{207}Pb^*/^{235}U$) and $^{207}Pb^*/^{206}Pb^*$. CONCH will (by default) plot the polygons in order of decreasing size, so that smaller polygons (i.e. more precise analyses) are plotted on top of, and are thus not obscured by, larger polygons. All analyses within a group will be displayed with the same polygon fill color, with each group displayed using a different fill color. As *x*- and *y*-axis uncertainties are not correlated on the Tera-Wasserburg Concordia diagram, analyses are displayed using conventional ±1σ-level *x*- and *y*-coordinate "error-bars", with the group fill color within the circle at the at error-bar intercepts. Only *y* error bars are shown on the Linearized Gaussian diagram, with the group fill color shown within a circle at the mid-point of the error-bar.

The Gaussian-summation probability density diagram displays two probability density curves, the first of which includes all (including discordant) analyses, and the second of which includes only concordant analyses (i.e. $^{206}Pb^*/^{238}U$ date within uncertainty of $^{207}Pb^*/^{206}Pb^*$ date at ±2σ uncertainty level, or within a User-specified percentage of concordance). To generate these curves, CONCH uses the Gaussian distribution probability density function:

$$G(i) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}} \qquad (9)$$

where x_i is the analysis ratio, μ is the mean and σ the analysis standard deviation. Conventionally, the area under probability curves sums to unity. However, as the probability density diagram is mainly used qualitatively, to compare relative probabilities (with an arbitrary or no *y*-axis scale), and in order to minimize rounding errors that result in steps in the curve, the curves have been rescaled so that the maximum peak height of the second (concordant analyses only) curve is a fixed percentage (User-defined in the Plot Options dialog) of the *y*-axis length. Because the probability density curves are constructed iteratively by summing values for each analysis at points along the probability density curve, the diagram commonly takes some seconds to generate, so the calculated age range is initially subdivided into a comparatively small default bin size of 100. The bin size can be increased, via the "Probability Plot Edit" dialog (Fig. 14), to generate smoother probability density curves, once other aspects of the diagram have been finalized. Best results are usually obtained with bin sizes of 400 or 500.

The Linearized Gaussian diagram is equivalent to plotting analyses on "Normal Probability Paper". The cumulate probability density function will plot as a straight line on such probability paper, enabling the assumption of a Gaussian distribution of data about a mean value (i.e. individual analyses about a mean $^{207}Pb^*/^{206}Pb^*$, $^{206}Pb^*/^{238}U$ or $^{207}Pb^*/^{235}U$ $^{208}Pb/^{232}Th$ date) to be assessed. In practice, this diagram has proven to be remarkably useful for the investigation of the causes behind rare examples in which a group of $^{207}Pb^*/^{206}Pb^*$, $^{206}Pb^*/^{238}U$, $^{207}Pb^*/^{235}U$ or $^{208}Pb^*/^{232}Th$ analyses do not show a Gaussian

distribution about a mean value. A common cause of skewed distributions is the preferential loss of radiogenic-Pb from high-U analysis sites; on the Linearized Gaussian diagram, this manifests as a "tilted conical" arrangement of analyses, whereby analyses from higher-U sites and with smaller uncertainties, the uncertainty bars of which form a "cone", are concentrated at the lower ("tilted") right-hand side of the plot. To generate the Linearized Gaussian diagram, CONCH uses *Benard's approximation* to calculate a median rank (MR), as a percentage, for each point:

$$MR = \frac{x_i - 0.3}{n + 0.4} \qquad (10)$$

where x_i is the analysis ratio and n is the total number of analyses.

An "Add Data" button, located along the bottom of each plot window, enables data from a "Processed Data" output file to be included and processed with data displayed on any of the diagrams. CONCH will match the sample labels of analyses within a "Processed Data" output file with that specified in the "Processed Data" file "active label" textbox in the Set-up dialog or, if the displayed data is from a SHRIMP output (raw data) file, with that specified in the "sample label" textbox in the Standards dialog. If no label was specified in these textboxes, CONCH will display a dialog enabling the User to provide an "active" label. If the dialog textbox is left null, all data in the file will be read and displayed.

Switching between any of the diagrams, assessment and editing of the group assignment and generation of the processed data file, is readily achieved using buttons located in the diagram windows and on the Report Sheet. Group labels may be added adjacent to analyses on the diagrams using the Summary button. These labels include a comma-delimited list of the analysis labels within the group, the group date and its uncertainty. The diagrams generated by CONCH may be imported into any graphics program to produce publication-quality figures.

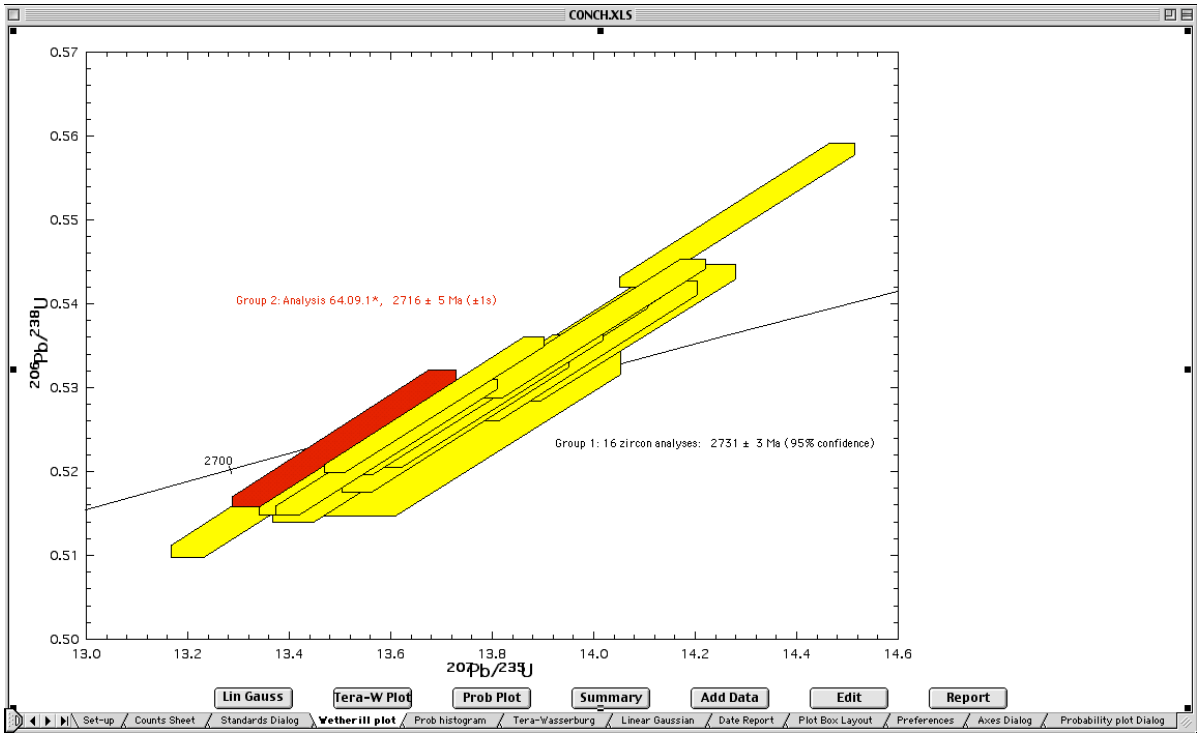

Fig. 9.1. The Wetherill Sheet.

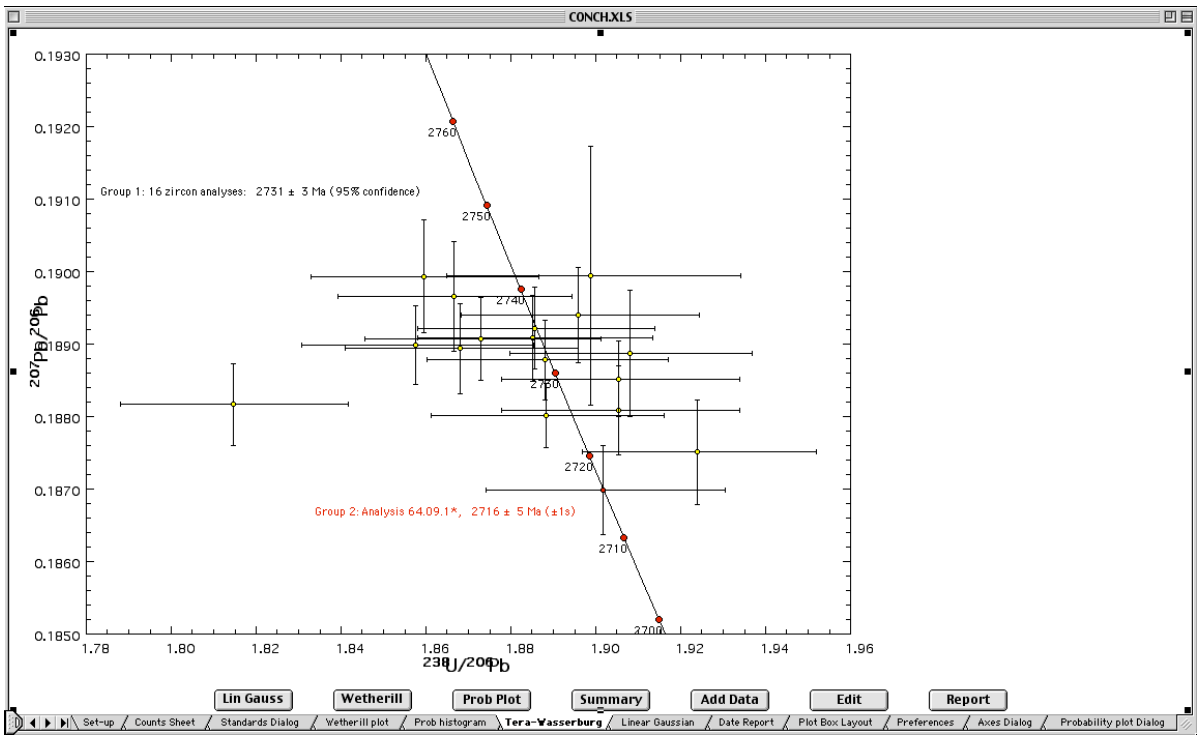

Fig. 9.2. The Tera-Wasserburg Sheet.

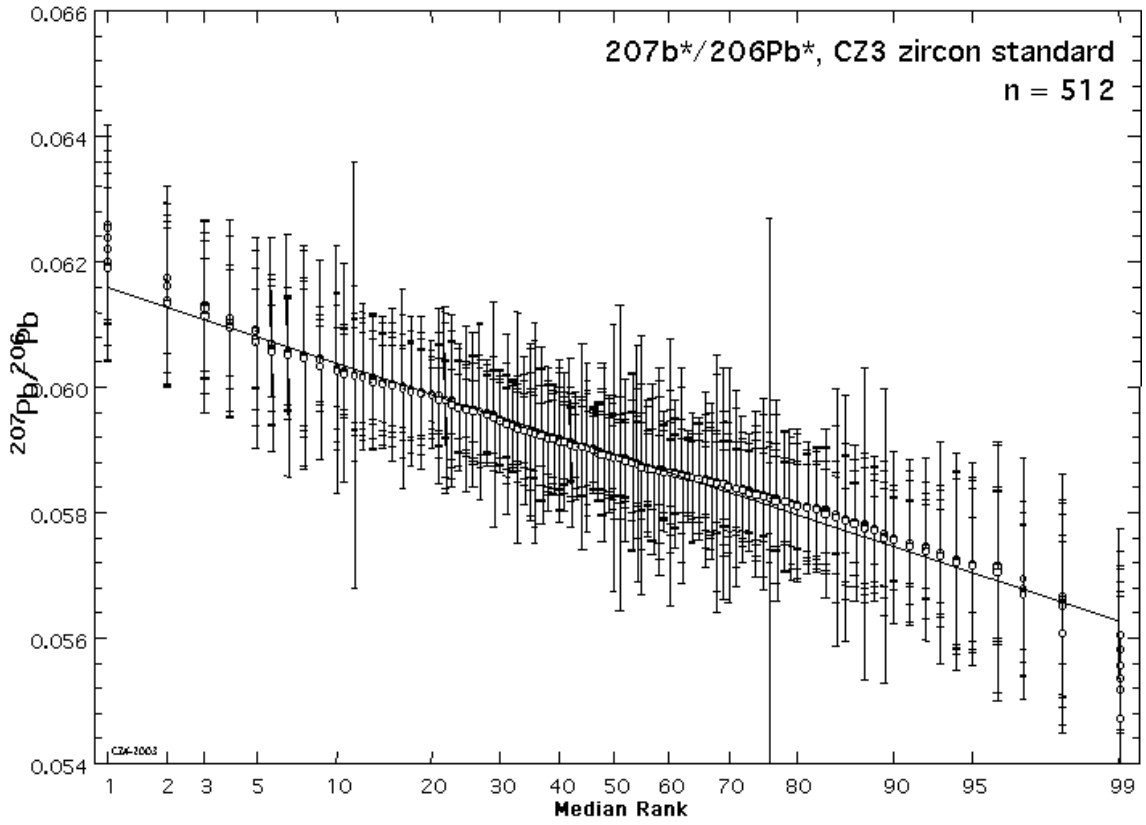

Fig. 9.3. An example of a Linearized Gaussian diagram generated by CONCH. The data shown are $^{207}Pb/^{206}Pb$ ratios obtained for analyses of the CZ3 zircon standard on the SHRIMP-2A during 2003.

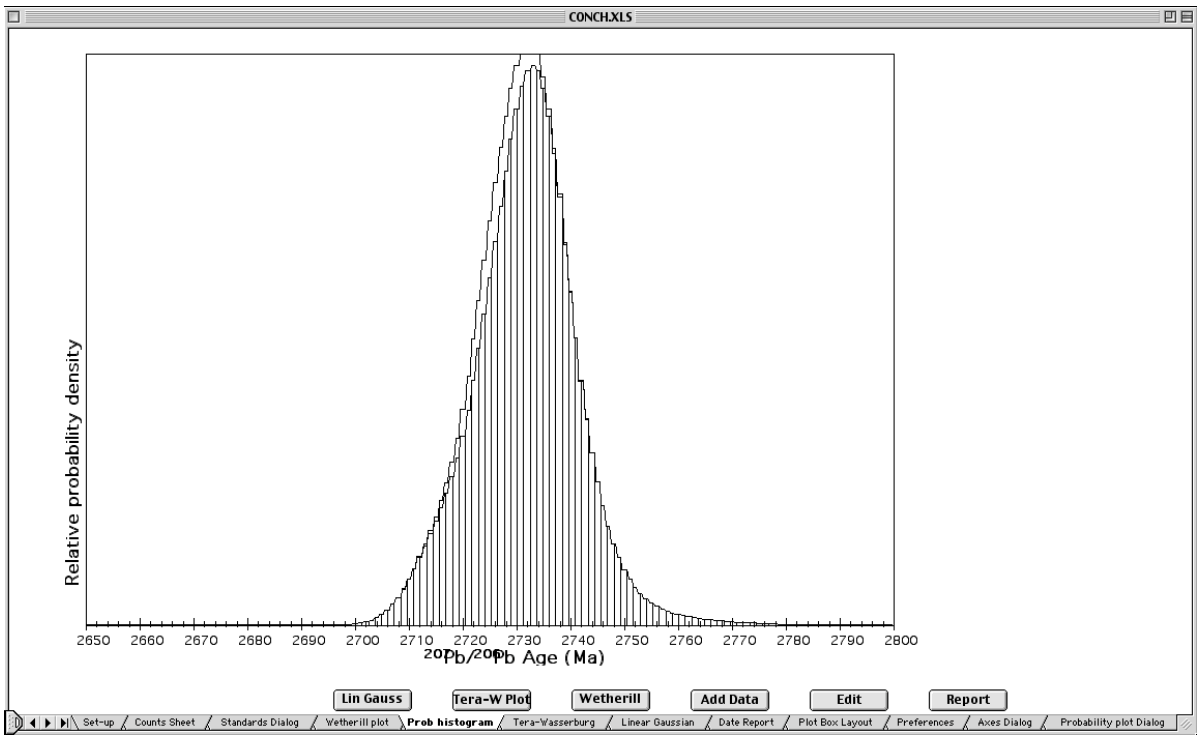

Fig. 9.4. The Gaussian-summation probability density Sheet.

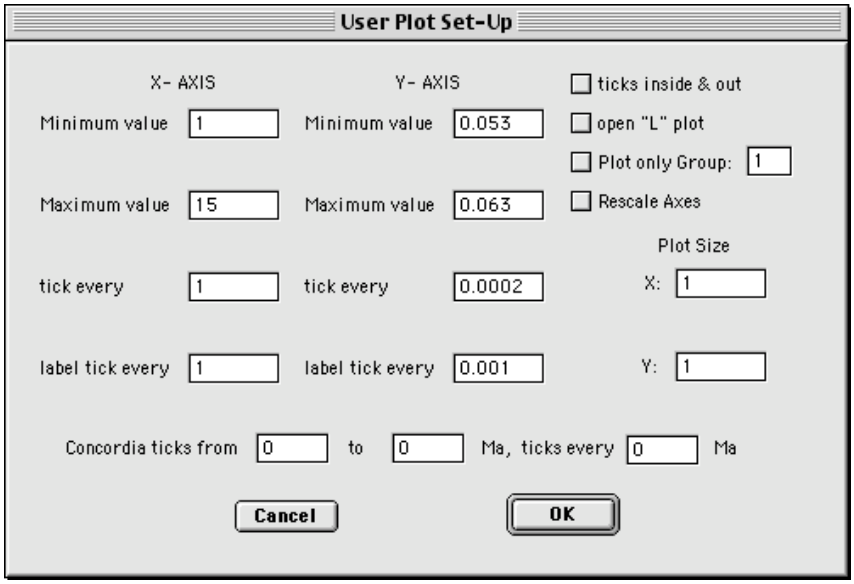

Fig. 9.5. The Plot Edit dialog.

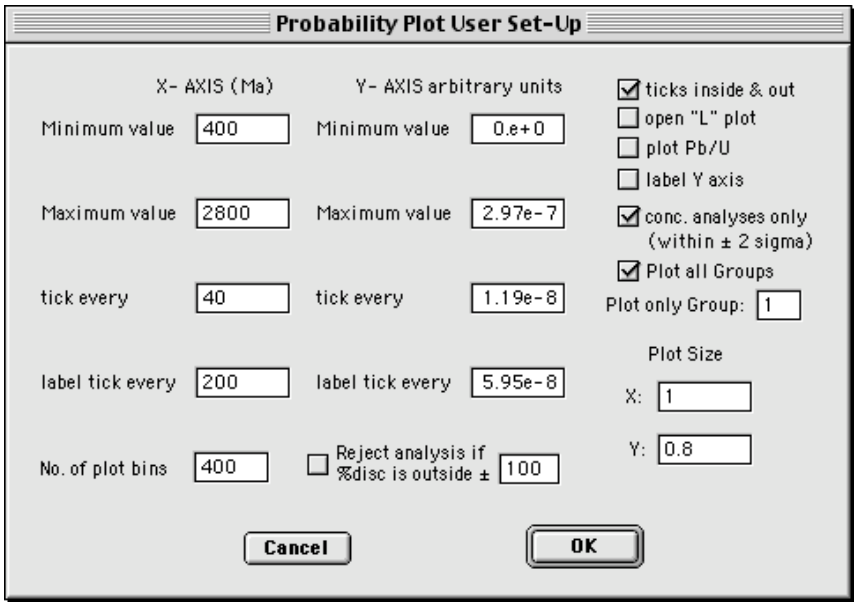

Fig. 9.6. Gaussian-summation probability density diagram Edit dialog.

Table 9.1. List of controls in the User Plot Set-up dialog called from Wetherill, Tera-Wasserburg and Linearized Gaussian diagram sheets, with a description of their functions.

Control label	Control type	Function
X-AXIS: Minimum value	Editbox	Displays the current *x*-axis minimum value displayed on the diagram from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets), for editing by the User prio to replotting
X-AXIS: Maximum value	Editbox	Displays the current *x*-axis maximum value displayed on the diagram from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets), for editing by the User prio to replotting
X-AXIS: tick every	Editbox	Displays the current *x*-axis tick interval value displayed on the diagram from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets), for editing by the User prio to replotting
X-AXIS: label tick every	Editbox	Displays the current *x*-axis tick interval value at which an axis label is displayed, on the diagram from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets) for editing by the User prior to replotting
Y-AXIS: Minimum value	Editbox	Displays the current *y*-axis minimum value displayed on the diagram from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets), for editing by the User prio to replotting
Y-AXIS: Maximum value	Editbox	Displays the current *y*-axis maximum value displayed on the diagram from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets), for editing by the User prio to replotting
Y-AXIS: tick every	Editbox	Displays the current *y*-axis tick interval value displayed on the diagram from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets), for editing by the User prio to replotting
Y-AXIS: label tick every	Editbox	Displays the current *y*-axis tick interval value at which an axis label is displayed, on the diagram from which the dialog was called (either the Wetherill or Tera-Wasserburg diagram sheets), for editing by the User prior to replotting
Concordia ticks from	Editbox	Displays the minimum date, in Ma, that will be displayed adjacent to a tick on the Concordia curve on the diagram from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets), for editing by the User prior to replotting
Concordia ticks from: to:	Editbox	Displays the maximum date, in Ma, that will be displayed adjacent to a tick on the Concordia curve on the diagram from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets), for editing by the User prior to replotting
Concordia ticks from: to: ticks every: Ma	Editbox	Displays the tick interval, in Ma, at which ticks and labels will be displayed on the Concordia curve on the diagram from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets), for editing by the User prior to replotting
Ticks inside & out:	Checkbox	If checked, specifies that ticks on the *x*-axis and *y*-axis are to be displayed on both sides of the axes (rather than only on the inside, as in the default case) on the diagram sheet from which the dialog was called (eithe the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets) when the "OK" button is selected and the diagram is redrawn
Open "L" plot:	Checkbox	If checked, specifies that single *x*-axis and *y*-axis (i.e. "L"-shape, rather than the default "box") are to be displayed on the diagram sheet from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets) when the "OK" button is selected and the diagram is redrawn
Plot only Group:	Checkbox	If checked, specifies that only analyses belonging to the Age group specified in the "Plot only Group" editbox, are to be displayed on the diagram sheet from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets) when the "OK" button is selected and the diagrar is redrawn
Plot only Group:	Editbox	If the Plot only Group checkbox is checked, only analyses belonging to the Age group equivalent to that specified in the "Plot only Group" editbox are to be displayed on the diagram sheet from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets) when the "OK" button is selected and the diagram is redrawn
Rescale Axes:	Checkbox	If checked, specifies that the *x*-axis and *y*-axis ranges and tick intervals are to be automatically recalculated (i.e. entries in the *x*-axis and *y*-axis editboxes are ignored) and displayed on the diagram sheet from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets) when the "OK" button is selected and the diagram is redrawn
Plot Size: X:	Editbox	Specifies the value by which the *x*-axis length is rescaled and displayed on the diagram sheet from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets) when the "OK" button is selected and the diagram is redrawn
Plot Size: Y:	Editbox	Specifies the value by which the *y*-axis length is rescaled and displayed on the diagram sheet from which the dialog was called (either the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets) when the "OK" button is selected and the diagram is redrawn
OK:	Button (default)	Closes the User Plot Set-up dialog, returns to We the calling (Wetherill, Tera-Wasserburg or Linearized Gaussian) sheets, and uses the values in the edit box to replot the diagram
Cancel:	Button	Closes the User Plot Set up dialog and returns to the diagram sheet from which the dialog was called (eithe the Wetherill, Tera-Wasserburg or Linearized Gaussian diagram sheets)

Table 9.2. List of controls in the User Plot Set-up dialog called from the Gaussian-summation probability density diagram sheets, with a description of their functions.

Control label	Control type	Function
X-AXIS: Minimum value	Editbox	Displays the current *x*-axis minimum value displayed on the Gaussian-summation probability density diagram, for editing by the User prior to replotting
X-AXIS: Maximum value	Editbox	Displays the current *x*-axis maximum value displayed on the diagram from which the dialog was called (either the Wetherill or Tera-Wasserburg diagram sheets), for editing by the User prior to replotting
X-AXIS: tick every	Editbox	Displays the current *x*-axis tick interval value displayed on the Gaussian-summation probability density diagram, for editing by the User prior to replotting
X-AXIS: label tick every	Editbox	Displays the current *x*-axis tick interval value at which an axis label is displayed on the Gaussian-summation probability density diagram, for editing by the User prior to replotting
Y-AXIS: Minimum value	Editbox	Displays the current *y*-axis minimum value displayed on the Gaussian-summation probability density diagram, for editing by the User prior to replotting
Y-AXIS: Maximum value	Editbox	Displays the current *y*-axis maximum value displayed on the Gaussian-summation probability density diagram, for editing by the User prior to replotting
Y-AXIS: tick every	Editbox	Displays the current *y*-axis tick interval value displayed on the Gaussian-summation probability density diagram, for editing by the User prior to replotting
Y-AXIS: label tick every	Editbox	Displays the current y-axis tick interval value at which an axis label is displayed on the Gaussian-summation probability density diagram, for editing by the User prior to replotting
No. of plot bins:	Editbox (default value =100)	Displays the number of plot bins used to calculate the Gaussian-summation probability density curve, for editing by the User prior to replotting. For a smooth curve, a value of c. 400-500 is recommended.
Reject analysis if %disc is outside ±:	Checkbox	If checked, tests that the concordance of each analysis is within the value specified in the "Reject analysis if %disc is outside ±" editbox. If this is the case, the analysis is used to calculate the Gaussian-summation probability density curve and displayed on the Gaussian-summation probability density diagram, when the "OK" button is selected and the diagram is redrawn. If not, the analysis is not used in calculating the curve.
Reject analysis if %disc is outside ±:	Editbox	If the "Reject analysis if %disc is outside ±" checkbox is checked, tests that the concordance of each analysis is within (analysis is more concordant than) the value specified in the editbox. If this is the case, the analysis is used to calculate the Gaussian-summation probability density curve and displayed on the Gaussian-summation probability density diagram, when the "OK" button is selected and the diagram is redrawn. If not, the analysis is not used in calculating the curve.
Ticks inside & out:	Checkbox	If checked, specifies that ticks on the *x*-axis and *y*-axis are to be displayed on both inside and outside of the axes (rather than only on the inside, as in the default case) on the Gaussian-summation probability density diagram sheet when the "OK" button is selected and the diagram is redrawn
Open "L" plot:	Checkbox	If checked, specifies that only single *x*-axis and *y*-axis (in "L"-shape, rather than the default "box") are to be displayed on the Gaussian-summation probability density diagram sheet when the "OK" button is selected and the diagram is redrawn
Plot Pb/U:	Checkbox	If checked, specifies that the Gaussian-summation probability density curve to be displayed on the Gaussian-summation probability density diagram sheet is for Pb*/U values on the *x*-axis when the "OK" button is selected and the diagram is redrawn. The default curve is for $^{207}Pb^*/^{206}Pb^*$.
Label Y axis:	Checkbox	If checked, specifies that labels are *y*-axis on the Gaussian-summation probability density diagram sheet are to be scaled and labeled when the "OK" button is selected and the diagram is redrawn. The default is that the *y*-axis is not labeled.
Plot all Groups:	Checkbox	If checked, specifies that all analyses are to be displayed on the Gaussian-summation probability density diagram sheet when the "OK" button is selected and the diagram is redrawn
Plot only Group:	Editbox	If the Plot only Group checkbox is not checked, only analyses belonging to the Age group equivalent to that specified in the "Plot only Group" editbox are to be displayed on the Gaussian-summation probability density diagram sheet when the "OK" button is selected and the diagram is redrawn
Plot Size: X:	Editbox	Specifies the value by which the *x*-axis length is rescaled and displayed on the diagram sheet from which the dialog was called (either the Wetherill or Tera-Wasserburg diagram sheets) when the "OK" button is selected and the diagram is redrawn
Plot Size: Y:	Editbox	Specifies the value by which the *y*-axis length is rescaled and displayed on the diagram sheet from which the dialog was called (either the Wetherill or Tera-Wasserburg diagram sheets) when the "OK" button is selected and the diagram is redrawn
OK:	Button (default)	Closes the Gaussian-summation probability density diagram User Set-up dialog, returns to the Gaussian-summation probability density diagram sheet and uses the values in the Gaussian-summation probability density diagram User Set-up dialog edit boxes to replot the diagram
Cancel:	Button	Closes the Gaussian-summation probability density diagram User Set up dialog and returns to the Gaussian-summation probability density diagram sheet

10. Report types

Depending on the analysis type specified in the Set-up dialog, several different Report types may be generated by CONCH. All Report types are initially written to the Report Sheet (see Fig. 3.2 for an example). The writing to disk of a Report text file, that may be read using any spreadsheet program, may be initiated by the "Save As" dialog, which is summoned using the "Report File" button on the Report Sheet.

As CONCH input files are "*text only*" (tab-delimited text) files, output files should always be saved as the "*Text Only*" file type when saving a CONCH-generated output file.

10.1 The Generalized Report type

The Generalized Report type may be selected using the Counts/Ratios analysis type in the Set-up dialog. This Report and output file type may be generated from any readable ion-microprobe output (raw data) file. It is not necessary to identify any of the species in the raw data input file using a run-table for this report type. However, if the mass species are not identified, either by use of a run-table or from a SHRIMP ".sq" file type in which the mass species are identified, then (because the background species is not identified) background corrections cannot be made to the count rates. Not identifying a background species (or alternatively, identification in the Run-table dialog of the background species as a mass species for processing) may be useful when monitoring of background count rates during an analysis session is required. The Generalized Report tabulates count rates (as counts/s), corrected for background counts provided a background species has been identified, for all species. Also tabulated are ratios of the count rates, using a denominator mass that may be specified in the "Denominator-Y" textbox of the Run-table dialog, the ratio's uncertainty based on counting statistics, and its D value (see equation 8). If no denominator has been specified (i.e. if the "OK" button on the Run-table dialog has not been used), the default denominator is the first species of each analysis read from the input file. Standard analyses are tabulated (in the order that they were read from the input file) separately, and averages, weighted means and observed and expected uncertainties for ratios obtained for standards are also listed. Next, each standard and unknown analysis, with averages, weighted means and observed and expected uncertainties for ratios obtained for all analyses, are tabulated in analysis order. The REE/Trace element, ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr and ^{60}Fe-^{60}Ni report types are derivatives of the Generalized Report type. The ^{26}Al-^{26}Mg, ^{53}Mn-^{53}Cr and ^{60}Fe-^{60}Ni report types will also tabulate mass fractionation-corrected and normalized ^{26}Mg/^{24}Mg, ^{53}Cr/^{52}Cr and ^{60}Ni/^{62}Ni ratios, their averages, weighted means and observed and expected uncertainties. The ^{25}Mg/^{24}Mg, ^{50}Cr/^{52}Cr and ^{60}Ni/^{62}Ni ratios used to correct for mass fractionation, and the ^{26}Mg/^{24}Mg, ^{53}Cr/^{52}Cr and ^{60}Ni/^{62}Ni normalization ratios, are displayed, and may be modified, in the Run-table dialog when these analysis types are chosen.

10.2 The Date Report type and User-editing of age groups

The Date Report is the report type written to the Report Sheet for Zircon, Monazite, Xenotime, Titanite/Perovskite, Baddeleyite/Common Pb and Th–U Disequilibrium analysis types. The layout of the Date Report type (see Fig. 10.1) has been designed to facilitate User-editing of age groups and printing. Because analyses belonging to different groups are displayed in different fill colors on the diagrams, the Date Report on the Report Sheet and the Wetherill Concordia, Tera-Wasserburg Concordia, Linearized Gaussian and Gaussian-summation probability density diagrams are intended to be used together, so that the consequences of reassigning analyses among age groups is evident from examination of these diagrams. Depending on the "Group by" option selected in the Set-up dialog, analyses will be assigned to ^{207}Pb/^{206}Pb, ^{207}Pb*/^{206}Pb*, ^{206}Pb*/^{238}U, ^{207}Pb*/^{235}U or ^{208}Pb*/^{232}Th age groups, based on the chi-square and D threshold parameters specified in the Set-up dialog that are used to define these groups. Analyses may be manually redistributed amongst age groups by inserting an integer corresponding to the new age group in the cell adjacent to, and to the right of, the analysis (column 14) to be moved on the Report Sheet, moving the cursor outside the cell, and selecting the "Recalc" button on the Report Sheet. The Date Report will be updated on the Report Sheet, with the analysis reassigned to the new age group. The validity of the move may be assessed by examination of the analysis's D value and the new group's chi-value on the revised Report Sheet. The consequences of the reassignment may be examined graphically on the Wetherill Concordia, Tera-Wasserburg Concordia, Linearized Gaussian and Gaussian-summation probability density diagrams by using the

"Plot" button on the Report Sheet. A "Processed Data" output file can be written to disk using the "Files" button on the Report Sheet (ensure that the "*Text Only*" output file type is selected).

DATEREPORT- 204Common-Pb Correction method Analyses grouped by 207Pb*/206Pb*

Group No. 1

Sample	206/238	+/-	diff	207/235	+/-	diff	208/232	+/-	diff	207/206	+/-	diff
64.02.1	0.528	0.008	-0.18	13.742	0.226	-0.2	0.0984	0.0016	0.29	0.18878	0.00055	0.06
64.03.1	0.534	0.008	0.57	13.974	0.231	0.78	0.1003	0.0016	1.41	0.18965	0.00076	1.17
64.04.1	0.537	0.008	0.88	13.995	0.225	0.89	0.0987	0.0016	0.47	0.18899	0.00054	0.43
64.05.1	0.551	0.009	2.38	14.283	0.232	2.07	0.0986	0.0016	0.42	0.18817	0.00056	-1
64.06.1	0.529	0.008	-0.09	13.794	0.224	0.02	0.0982	0.0016	0.16	0.18922	0.00057	0.8
64.07.1	0.532	0.008	0.34	13.88	0.226	0.39	0.1004	0.0016	1.49	0.18907	0.00057	0.54
64.08.1	0.522	0.008	-0.87	13.599	0.23	-0.8	0.0987	0.0016	0.48	0.18887	0.00087	0.14
64.10.1	0.534	0.008	0.52	13.91	0.226	0.52	0.0985	0.0016	0.37	0.18894	0.00062	0.3
64.12.1	0.537	0.008	0.83	14.051	0.228	1.11	0.1001	0.0015	1.35	0.18993	0.00078	1.5
64.14.1	0.525	0.01	-0.46	13.744	0.308	-0.14	0.0931	0.0019	-2.52	0.18994	0.00178	0.67
64.15.1	0.529	0.008	-0.08	13.786	0.223	-0.01	0.0959	0.0015	-1.32	0.18908	0.0006	0.54
64.16.1	0.528	0.008	-0.19	13.685	0.216	-0.46	0.0981	0.0015	0.1	0.18801	0.00045	-1.54
64.17.1	0.526	0.008	-0.46	13.728	0.224	-0.26	0.0969	0.0015	-0.63	0.1894	0.00065	0.98
64.18.1	0.523	0.008	-0.79	13.56	0.22	-1	0.0974	0.0015	-0.3	0.18808	0.00061	-1.05
64.19.1	0.523	0.008	-0.79	13.592	0.218	-0.87	0.0963	0.0015	-1.04	0.18852	0.00052	-0.41
64.20.1	0.518	0.008	-1.47	13.382	0.215	-1.83	0.0964	0.0015	-0.97	0.18751	0.00072	-1.67

n=16		Mean	Exp.s.e.	Obs.s.e.	Age(Ma)	Exp.s.e.		Obs.s.e.	
206/238									
	unweighted	0.52965	0.00209	0.00196					
	weighted	0.52952	0.00207	0.00195	2739.4	8.7	-8.7	8.2	-8.2
	calibrated		0.00337	0.0033		14.2	-14.2	13.9	-13.9
	95%confidence		0.00718	0.007		30.2	-30.3	29.5	-29.7
chi-sq:	0.83								
207/235									
	unweighted	13.7941	0.05762	0.05489					
	weighted	13.7886	0.0569	0.05554	2735.3	3.9	-3.9	3.8	-3.8
	calibrated		0.0895	0.0887		6.1	-6.2	6.1	-6.1
	95%confidence		0.1908	0.189		13	-13.2	12.9	-13.1
chi-sq:	0.9								
208/232									
	unweighted	0.09788	0.00039	0.00047					
	weighted	0.09793	0.00039	0.00044	1888.4	7.2	-7.2	8	-8
	calibrated		0.001	0.001		18.7	-18.7	19	-19.1
	95%confidence		0.0022	0.0022		39.9	-39.9	40.6	-40.7
chi-sq:	1.17								
207/206									
	unweighted	0.18889	0.00019	0.00017					
	weighted	0.18875	0.00015	0.00015	2731.3	1.3	-1.4	1.3	-1.4
	95%confidence		0.0003	0.0003		2.9	-2.9	2.9	-2.9
chi-sq:	0.93								

Student's t for 16 analyses: 2.13

GroupNo. 2

Sample	206/238	+/-	diff	207/235	+/-	diff	208/232	+/-	diff	207/206	+/-	diff
64.09.1	0.524	0.008	0	13.508	0.221	0	0.0989	0.0016	0	0.18699	0.00061	0

n=1		Mean	Exp.s.e.	Obs.s.e.	Age(Ma)	Exp.s.e.		Obs.s.e.	
206/238									
	unweighted	0.52965	0.00209	0.00817					
	weighted	0.52395	0.00817	0.00817	2715.9	34.5	-34.6	34.5	-34.6
	calibrated		0.00858	0.00858		36.2	-36.4	36.2	-36.4
207/235									
	unweighted	13.7941	0.05762	0.22055					
	weighted	13.5082	0.2205	0.22055	2715.9	15.3	-15.6	15.3	-15.6
	calibrated		0.2307	0.2307		16	-16.3	16	-16.3
208/232									
	unweighted	0.09788	0.00039	0.00158					
	weighted	0.09892	0.00158	0.00158	1906.7	29	-29	29	-29
	calibrated		0.0018	0.0018		33.8	-33.9	33.8	-33.9
207/206									
	unweighted	0.18889	0.00019	0.00061					
	weighted	0.18699	0.00061	0.00061	2715.8	5.4	-5.4	5.4	-5.4

File	8-206Pb/238U%	4-208Pb/232Th%	standards	unknowns	cal.slope
DesktopFolder: data file	1.418	2.71	8	18	2

Fig. 10.1. The Report Sheet showing an example of a Date Report.

Acknowledgements

Thanks to R. Adam Frew, Eric Thern and Andrea Biondo for stimulating discussions and capable assistance with all aspects of SHRIMP analytical work, and also Kenny Sia Tze Foo, who diligently undertook a Monte Carlo investigation of uncertainty propagation in U-Pb dating as part of a 3rd year student project within the School of Physical Sciences, Curtin University of Technology.

References

Black, L.P. and Jagodzinski, E.A., 2003. Importance of establishing sources of uncertainty for the derivation of reliable SHRIMP ages. Australian Journal of Earth Sciences, Volume 50, Issue 4, p. 503-512.

Claoué-Long, J.C., Compston, W., Roberts, J. and Fanning, C.M., 1995, Two Carboniferous ages: a comparison of SHRIMP zircon dating with conventional zircon ages and $^{40}Ar/^{39}Ar$ analyses. Geochronology Time Scales and Global Stratigraphic Correlation, SEPM Special Publication No. 54, p. 3-21

Compston, W., Williams, I. S., and Meyer, C., 1984, U–Pb geochronology of zircons from lunar breccia 73217 using a sensitive high mass-resolution ion microprobe: Journal of Geophysical Research, v. 89, p. B252–B534.

Compston, W., 1999. Geological age by instrumental analysis: the 29th Hallimond Lecture. Mineralogical Magazine, Volume 63, Issue 3, p. 297-311.

Compston, W., 2001. Effect of Pb loss on the ages of reference zircons QGNG and SL13, and of volcanic zircons from the Early Devonian Merrions and Turondale Formations, New South Wales. Australian Journal of Earth Sciences, Volume 48, p. 797-803.

Cumming, G. L., and Richards, J. R., 1975, Ore lead ratios in a continuously changing Earth: Earth and Planetary Science Letters, v. 28, p. 155–171.

Fletcher, I.R., Rasmussen, B., and McNaughton, N.J., 2000. SHRIMP U-Pb geochronology of authigenic xenotime and its potential for dating sedimentary basins. Australian Journal of Earth Sciences, Volume 47, p. 845-859.

Kinny, P.D., 1997. Users guide to Th-U-Pb dating of titanite, perovskite, monazite and baddeleyite using the WA SHRIMP. School of Physical Sciences, Curtin University of Technology, Report No. SPS 693/1997/AP72, 21 pp.

Moroney, M.J. 1984. Facts from Figures. 2th edition. Pengiun Books Ltd., Middlesex, England, 472pp.

Steiger, R.H. and Jaeger, E., 1977. Subcommision on geochronology: convention on the use of decay constants in geo- and cosmochronology. Earth and Planetary Science Letters 36, p. 359-362.

Stern, R.A., and Amelin, Y., (2003). Assessment of errors in SIMS zircon U-Pb geochronology using a natural zircon standard and NIST SRM 610 glass. Chemical Geology 197, p. 111-142.

Stern, R.A., and Sanborn, N., 1998. Monazite U-Pb and Th-Pb geochronology by high-resolution secondary ion mass spectrometry. In: Radiogenic Age and Isotopic Studies: Report 11; Geological Survey of Canada, Current Research, 1998-F, p.1-18.

Wetherill, G.W., 1956, Discordant uranium-lead ages: Transactions of the American Geophysical Union, v. 37, p. 320–6.

Williams, I.S., and Hergt, J.M., 2000. U-Pb dating of Tasmanian dolerites: a cautionary tale of SHRIMP analysis of high-U zircon. In: Woodhead, J.D., Hergt, J.M., and Noble, W.P., (eds.), "Beyond 2000: New Frontiers in Isotope Science", pp. 185-188. School of Earth Sciences, University of Melbourne, Melbourne.

Williams, I. S., Buick, I. S., Cartwright, I., 1996. An extended episode of early Mesoproterozoic metamorphic fluid flow in the Reynolds Range, central Australia. Journal of Metamorphic Geology 14, p. 29–47.

Appendix 1. Example files included with CONCH

The text file labeled "Calibration File" and all tab-delimited text files with names ending in ".data", "PbPbtable" and ".PbUtable" were output by CONCH. They may be opened and examined using Excel and may be read for re-plotting by CONCH; check the "Processed Data File" checkbox and select the appropriate file format using the "In/Out file type" check-boxes in the Set-up dialog.

The "PbPbtable" input file provides a convenient way for processed U-Pb geochronology data generated by means other than CONCH to be entered into CONCH for processing and plotting. The simplest way to achieve this is to open the "PbPbtable" example file provided, replace the labels, $^{207}Pb^*/^{206}Pb^*$, $\pm 1\sigma$ uncertainty, $^{206}Pb^*/^{238}U$, $\pm 1\sigma$ uncertainty, $^{207}Pb^*/^{235}U$, $\pm 1\sigma$ uncertainty column entries with those to be processed and plotted, and use "Save As.." to save a copy of the file as "*Text Only*". This file may then be input into CONCH for grouping and plotting.

Warning: Excel may add strings of hidden characters to the ends of files it saves. This may render a file unreadable by CONCH. If CONCH can't read a file after it has been opened and saved as "*Text Only*" by Excel, reopen the file using a Text Editor, delete any extra characters at the end of the file and resave a copy of the file as a "*Text Only*" file type.

1. zircon: this SHRIMP output file contains typical analytical data obtained on zircon during a single analysis session. It includes 12 analyses of the CZ3 standard and data obtained on two samples labeled "00" (28 analyses) and "02" (9 analyses).

2. zircon.data: this CONCH output file contains processed analytical data read from the input file: "zircon".

3. zircon.PbPbtable: this CONCH output file contains analytical data read by CONCH from the example input file: "zircon", processed and output in PbPbtable format. To read this file with CONCH, select the Processed Data File and PbPb table file type options in the Set-up dialog.

4. zircon.PbUtable: this CONCH output file contains analytical data read by CONCH from the example input file: "zircon", processed and output in PbUtable format. To read this file with CONCH, select the Processed Data File and PbU table file type options in the Set-up dialog.

5. monazite: this SHRIMP output file contains typical analytical data obtained on monazite during a single analysis session. The Faraday Cup was used to protect the multiplier during acquisition, so the "Cup-In" option should be checked in the Preferences dialog. The data file includes 7 analyses of the MAD monazite standard (labeled "MAD") and 20 analyses of one sample labeled "64".

6. monazite.data: this CONCH output file contains processed analytical data read from the input file: "monazite" (plus one additional MAD standard analysis).

7. Calibration_File: this CONCH output file contains a compilation of processed analytical data obtained on session zircon standards. Additional processed standard data may be appended to the file using the "Calibration file" button located on the Standards dialog.

8. zircon runtable.txt: this text file is an example of CONCH's run-table file. It may be read using the "Load run-table" button on CONCH's Set-up dialog. It may also be modified to permanently store zircon run-table settings.

9. monazite runtable: this text file may be read using the "Load run-table" button on CONCH's Set-up dialog and displayed using the Run-table dialog.

10. xenotime runtable: a text file that may be read using the "Load run-table" button on CONCH's Set-up dialog.

Appendix 2. Input file formats

Examples of the ".op" and ".sq" ion-microprobe (SHRIMP) output file formats that may be read by CONCH are given below. For examples of the file formats output by CONCH that may also be read by CONCH, see the ".data", calibration, PbPbtable, and PbUtable example files provided with the CONCH software.

1. Example of the ".op" input file format (2 analyses; file ends with two CR's)

```
CZ3.1
13:42:04 13/ 2/2006
1
6
9
2.00   10.00  10.00  10.00  20.00  10.00  5.00   5.00   2.00
21     161    301    441    581    721
32     171    311    451    591    731
43     183    323    463    603    743
65     205    345    485    625    765
83     223    363    503    643    783
100    240    380    520    660    800
117    257    397    537    677    817
131    271    411    551    691    831
143    283    423    563    703    843
26490  25934  26155  26208  26011  26027
32     12     10     7      12     7
0      0      0      0      0      1
17598  17972  17724  17446  17496  16889
2672   2458   2414   2307   2407   2328
857    647    637    621    653    664
34204  34225  33807  33815  33910  33522
12074  12149  11896  12014  11799  11797
99438  99694  98031  97893  96786  97530
6716
943550 943095 945902 936297 937467 942227
4707684       4721532       4741407       4679759       4685120       4703224
4709023       4737971       4740403       4683751       4680000       4704811
4721274       4726703       4737552       4724206       4674131       4709853
9420501       9493477       9492684       9420764       9347935       9415469
4724424       4742659       4699744       4694180       4683671       4717644
2355672       2370573       2342115       2338744       2356320       2365348
2356264       2361689       2347173       2340875       2351785       2372084
943243 946081 937969 934401 937888 954011

TEM1
14:01:41 13/ 2/2006
1
6
9
2.00   10.00  10.00  10.00  20.00  10.00  5.00   5.00   2.00
22     162    302    442    582    722
33     173    313    453    593    733
45     185    325    465    605    745
66     206    346    486    626    766
84     224    364    504    644    784
101    241    381    521    661    801
118    258    398    538    678    818
132    272    412    552    692    832
144    284    424    564    704    844
23445  22986  23161  23000  22808  22645
6      6      5      8      7      11
0      1      0      0      0      0
2347   2328   2142   2225   2191   2244
441    436    435    453    500    524
553    549    569    549    612    699
6518   6568   6567   6663   6309   6554
20072  20399  20126  20115  19453  19790
17205  17201  17256  17282  16889  16777
6716
924373 927627 935739 947274 945641 951844
4599898       4646527       4679422       4693742       4701033       4773775
4608253       4656052       4659189       4671577       4705756       4767793
4626989       4662741       4656256       4669361       4686275       4769732
9260927       9380159       9394320       9401305       9431545       9626715
4607837       4690988       4690081       4697375       4715164       4820276
2301313       2354645       2349915       2373941       2356131       2401274
2294395       2359304       2351198       2384715       2371055       2404562
924160 930709 943626 948007 944979 957970
```

2. Example of the ".sq" input file format (2 analyses; file ends with two CR's)

```
CZ3.1
1:42:05 PM 13/ 2/2006
1
6
9
SPECIES
Zr2O   Pb204  Bkgrnd Pb206  Pb207  Pb208  U238   ThO248 UO254
primary beam = -3.3nA
2.00   10.00  10.00  10.00  20.00  10.00  5.00   5.00   2.00
21     161    301    441    581    721
32     171    311    451    591    731
43     183    323    463    603    743
65     205    345    485    625    765
83     223    363    503    643    783
100    240    380    520    660    800
117    257    397    537    677    817
131    271    411    551    691    831
143    283    423    563    703    843
26490  25934  26155  26208  26011  26027
32     12     10     7      12     7
0      0      0      0      0      1
17598  17972  17724  17446  17496  16889
2672   2458   2414   2307   2407   2328
857    647    637    621    653    664
34204  34225  33807  33815  33910  33522
12074  12149  11896  12014  11799  11797
99438  99694  98031  97893  96786  97530
6716
943550 943095 945902 936297 937467 942227
4707684       4721532       4741407       4679759       4685120       4703224
4709023       4737971       4740403       4683751       4680000       4704811
4721274       4726703       4737552       4724206       4674131       4709853
9420501       9493477       9492684       9420764       9347935       9415469
4724424       4742659       4699744       4694180       4683671       4717644
2355672       2370573       2342115       2338744       2356320       2365348
2356264       2361689       2347173       2340875       2351785       2372084
943243 946081 937969 934401 937888 954011

TEM1
2:01:42 PM 13/ 2/2006
1
6
9
SPECIES
Zr2O   Pb204  Bkgrnd Pb206  Pb207  Pb208  U238   ThO248 UO254
primary beam = -3.1nA
2.00   10.00  10.00  10.00  20.00  10.00  5.00   5.00   2.00
22     162    302    442    582    722
33     173    313    453    593    733
45     185    325    465    605    745
66     206    346    486    626    766
84     224    364    504    644    784
101    241    381    521    661    801
118    258    398    538    678    818
132    272    412    552    692    832
144    284    424    564    704    844
23445  22986  23161  23000  22808  22645
6      6      5      8      7      11
0      1      0      0      0      0
2347   2328   2142   2225   2191   2244
441    436    435    453    500    524
553    549    569    549    612    699
6518   6568   6567   6663   6309   6554
20072  20399  20126  20115  19453  19790
17205  17201  17256  17282  16889  16777
6716
924373 927627 935739 947274 945641 951844
4599898       4646527       4679422       4693742       4701033       4773775
4608253       4656052       4659189       4671577       4705756       4767793
4626989       4662741       4656256       4669361       4686275       4769732
9260927       9380159       9394320       9401305       9431545       9626715
```

```
4607837      4690988      4690081      4697375      4715164      4820276
2301313      2354645      2349915      2373941      2356131      2401274
2294395      2359304      2351198      2384715      2371055      2404562
924160 930709 943626 948007 944979 957970
```

3. Example of the run-table file format

An example of a CONCH run-table text file is given below. This file ("zircon runtable.txt" provided in the Examples folder) may be loaded using the "Load Run-table" button on the Set-up dialog, and it contents will be displayed in the Run-table dialog for User checking. CONCH uses the Analysis Type (Zircon, Monazite etc.) specified in the Set-up dialog to check the contents of the run-table file, so ensure that the correct Analysis Type is specified before loading a run-table from a file.

CONCH matches the strings (of variable length, up to the ":" character) on the left-hand side of each line to identify the line content and interprets the last 8 characters of the line (following the ":" character) as the content values, after removing spaces. Mass stations are loaded into the run-table in the order they are listed in the file. Up to 16 mass station strings may be specified in the file. Any parameters not specified in the file may be specified or entered using the Run-table dialog.

```
CONCH runtable 'right-justify values with spaces in last 8 characters of
line, and ensure you select the correct mineral in the Set-up dialog
before loading
mass 1:  Zr2O196
mass 2:    Pb204
mass 3:  Backgnd
mass 4:    Pb206
mass 5:    Pb207
mass 6:    Pb208
mass 7:     U238
mass 8:   ThO248
mass 9:    UO254
numerator x:   Pb206
denominator x:    U238
numerator y:   UO254
denominator y:    U238
standard calibration label:    cyyc
standard age (Ma):     564
standard 207Pb*/206Pb*:  0.05892
standard 208Pb*/206Pb*:  0.01745
standard 206Pb*/238U:  0.0914
standard 207Pb*/235U:  not used
standard 208Pb*/232Th:  not used
standard concentration label:    cxxc
standard calibration Th (ppm):  not used
standard trace element or U (ppm):     551
default common-Pb 204Pb/206Pb:    0.0625
default common-Pb 207Pb/206Pb:    0.9618
default common-Pb 208Pb/206Pb:   2.22855
```

Appendix 3. Data format of CONCH's "Processed Data" and "Standards Calibration" output file types

Each analysis within a "Processed Data" output file consists of the following tab-delimited entries (with ±1σ uncertainties for the preceding entry denoted by "+/-") in down-column order (columns may extend onto next page):

Analysis label
U/ppm
Th/ppm
Th/U
+/- (for analysis types other than monazite)
Total Pb/ppm
^{204}Pb counts
excess ^{204}Pb-corrected ^{204}Pb counts (analysis types other than monazite)
background counts
^{206}Pb counts
excess ^{204}Pb-corrected ^{204}Pb/^{206}Pb meas
+/-
^{207}Pb/^{206}Pb meas
+/-
^{208}Pb/^{206}Pb meas
+/-
first calibration ratio (for zircon, ^{206}Pb*/^{238}U)
+/-
^{206}Pb/^{238}U-0
+/-
^{207}Pb/^{235}U-0
+/-
^{208}Pb/^{232}Th-0
+/-
%conc-0
Age ^{206}Pb*/^{238}U-0
+/-
Age ^{207}Pb*/^{235}U-0
+/-
Age ^{207}Pb*/^{206}Pb*-0
+/-
Age ^{208}Pb*/^{232}Th-0
+/-
f^{206}Pb-4
+/-
^{207}Pb*/^{206}Pb*-4
+/-
^{208}Pb*/^{206}Pb*-4
+/-
^{204}Pb-corrected first calibration ratio
+/-
^{207}Pb*/U^{235}-4
+/-
^{208}Pb*/^{232}Th-4
+/-
%conc-4
Age ^{206}Pb*/^{238}U-4
+/-
Age ^{207}Pb*/^{235}U-4
+/-
Age ^{207}Pb*/^{206}Pb*-4
+/-
Age ^{208}Pb*/^{232}Th-4
+/-
f^{206}Pb-7
+/-
^{208}Pb*/^{206}Pb*-7
+/-
^{207}Pb-corrected first calibration ratio
+/-
^{206}Pb*/^{238}U-7
+/-
^{208}Pb*/^{232}Th-7
+/-
Age ^{206}Pb*/^{238}U-7
+/-
Age ^{208}Pb*/^{232}Th-7
+/-
f^{206}Pb-8
+/-
^{207}Pb*/^{206}Pb*-8
+/-
^{208}Pb-corrected first calibration ratio
+/-
^{206}Pb*/^{238}U-8
+/-
^{207}Pb*/^{235}U-8
+/-
%conc-8
Age ^{206}Pb*/^{238}U-8
+/-
Age ^{207}Pb*/^{235}U-8
+/-
Age ^{207}Pb*/^{206}Pb*-8
+/-
Assigned Age Group
Pb Sensitivity (counts/s/total Pb ppm)
Age (Ga) used to calculate common-Pb
Common ^{204}Pb/^{206}Pb
Common ^{207}Pb/^{206}Pb
Common ^{208}Pb/^{206}Pb
calculated Common ^{208}Pb/^{206}Pb
+/-
first calibration ratio (default for zircon is ^{206}Pb/^{238}U meas); for monazite this and the next two columns contain the ^{204}Pb counts and ^{204}Pb/^{206}Pb meas not corrected for excess ^{204}Pb and the uncalibrated ^{206}Pb/^{238}U-4 ratio)
second calibration ratio (for zircon the default is ^{238}U^{16}O/^{238}U meas; for monazite ^{238}U^{16}O$_2$/^{238}U^{16}O)
^{232}Th/^{238}U meas (^{232}Th/^{238}U^{16}O meas ^{232}Th^{16}O$_2$/^{238}U^{16}O meas and ^{232}Th^{16}O$_2$/^{232}Th meas for monazite)
^{90}Zr$_2$^{16}O/^{238}Umeas (^{138}La^{32}P^{16}O$_2$/^{238}U^{16}O for monazite)
standard ^{206}Pb*/^{238}U calib uncertainty (±1σ%)
standard ^{206}Pb*/^{232}Th calib uncertainty (±1σ%)
number of standard analyses used
^{206}Pb/^{238}U ratio uncorrected for high U/ppm for xenotime or ^{234}U^{16}O$_2$/^{238}U^{16}O for Th/U Disequil
Analysis time (hours and decimal seconds)
Input File Name (with path).

Throughout this contribution, an asterisk is used to indicate that the Pb abundance has been corrected for the common-Pb component and is the radiogenic component only (e.g. radiogenic component of ^{206}Pb is denoted by ^{206}Pb*). Entries ending in "meas" are background-corrected measured

(uncalibrated) ratios. Entries ending in "-0" are (background-corrected where possible) calibrated ratios, with no correction to the Pb abundance made for the presence of common-Pb. Entries ending in "-4", "-7" and "-8" are background-corrected calibrated ratios using the radiogenic-Pb abundance calculated using the ^{204}Pb-, ^{207}Pb- and ^{208}Pb-correction methods (Compston et al., 1984) respectively. f ^{206}Pb-4, f ^{206}Pb-7 and f ^{206}Pb-8 are 100 × (common ^{206}Pb/total ^{206}Pb) calculated using the ^{204}Pb-, ^{207}Pb- and ^{208}Pb-correction methods respectively. Dates and their uncertainties are in millions of years (Ma) except where otherwise indicated. The entries %conc-4, %conc-4, %conc-8 denote 100 × (^{206}Pb*/^{238}U age)/(^{207}Pb*/^{206}Pb* age), with the ratios ^{206}Pb*/^{238}U and ^{207}Pb*/^{206}Pb* calculated using the ^{204}Pb-, ^{207}Pb- and ^{208}Pb-correction methods respectively. The prefix "Common" denotes the ratio of the common-Pb ratios used for the common-Pb correction.

A "Standards Calibration" output file format, selected using the "Calibration File" button in the Standards dialog, enables standards data from each session to be appended to a preexisting standards data file, for the long-term monitoring of ion-microprobe performance and data quality and of different calibration options. The Standards Calibration output includes the following column entries in addition to those listed above (in down-column order):

The Standards Calibration output includes the following column entries in addition to those listed above (in down-column order):

analysis hydride (see below)
±
session average hydride
±
analysis excess ^{204}Pb counts (see below)
±
session average excess ^{204}Pb counts
±
$\log_e[^{206}Pb^*/^{238}U]$
$\log_e[^{238}U^{16}O/^{238}U]$
session average $\log_e[^{206}Pb^*/^{238}U]$
session average $\log_e[^{238}U^{16}O/^{238}U]$
slope of $\log_e[^{206}Pb^*/^{238}U] – \log_e[^{238}U^{16}O/^{238}U]$
y-intercept for $\log_e[^{206}Pb^*/^{238}U] – \log_e[^{238}U^{16}O/^{238}U]$
MSWD $\log_e[^{206}Pb^*/^{238}U] – \log_e[^{238}U^{16}O/^{238}U]$
slope of $\log_e[^{238}U^{16}O/^{238}U] – \log_e[^{232}Th^{16}O/^{238}U^{16}O]$
y-intercept for $\log_e[^{238}U^{16}O/^{238}U] – \log_e[^{232}Th^{16}O/^{238}U^{16}O]$
MSWD $\log_e[^{238}U^{16}O/^{238}U] – \log_e[^{232}Th^{16}O/^{238}U^{16}O]$
^{206}Pb/$^{238}U^{16}O$ meas
$\log_e[^{206}Pb^*/^{238}U^{16}O]$

(the following require $^{238}U^{16}O_2$ to have been included in the run-table)

$^{206}Pb^*/^{238}U^{16}O_2$
$^{238}U^{16}O_2/^{238}U^{16}O$ meas
$^{238}U^{16}O_2/^{238}U$ meas
$\log_e[^{238}U^{16}O_2/^{238}U^{16}O]$
slope of $\log_e[^{206}Pb^*/U] – \log_e[U^{16}O_2/U^{16}O]$
y-intercept $\log_e[^{206}Pb^*/^{238}U] – \log_e[^{238}U^{16}O_2/^{238}U^{16}O]$
MSWD for $\log_e[^{206}Pb^*/^{238}U] – \log_e[U^{16}O_2/U^{16}O]$
$\log_e[^{238}U^{16}O_2/^{238}U]$
slope of $\log_e[^{206}Pb^*/^{238}U] – \log_e[^{238}U^{16}O_2/^{238}U]$
y-intercept of $\log_e[^{206}Pb^*/^{238}U] – \log_e[^{238}U^{16}O_2/^{238}U]$
MSWD for $\log_e[^{206}Pb^*/^{238}U] – \log_e[^{238}U^{16}O_2/^{238}U]$
$\log_e[^{238}U^{16}O_2/^{238}U]$
$\log_e[^{206}Pb^*/^{238}U^{16}O]$
slope of $\log_e[^{206}Pb^*/^{238}U^{16}O] – \log_e[^{238}U^{16}O_2/^{238}U^{16}O]$
y-intercept $\log_e[^{206}Pb^*/^{238}U^{16}O] – \log_e[^{238}U^{16}O_2/^{238}U^{16}O]$
MSWD $\log_e[^{206}Pb^*/^{238}U^{16}O] – \log_e[^{238}U^{16}O_2/^{238}U^{16}O]$
$\log_e[^{238}U^{16}O/^{238}U]$
$\log_e[^{206}Pb^*/^{238}U^{16}O_2]$
slope of $\log_e[^{206}Pb^*/^{238}U^{16}O_2] – \log_e[^{238}U^{16}O/^{238}U]$
y-intercept $\log_e[^{206}Pb^*/^{238}U^{16}O_2] – \log_e[^{238}U^{16}O/^{238}U]$
MSWD $\log_e[^{206}Pb^*/^{238}U^{16}O_2] – \log_e[^{238}U^{16}O/^{238}U]$
$\log_e[^{238}U^{16}O_2/^{238}U^{16}O]$
$\log_e[^{206}Pb^*/^{238}U^{16}O_2]$
slope $\log_e[^{206}Pb^*/^{238}U^{16}O_2] – \log_e[^{238}U^{16}O_2/^{238}U^{16}O]$
y-intercept $\log_e[^{206}Pb^*/^{238}U^{16}O_2] – \log_e[^{238}U^{16}O_2/^{238}U^{16}O]$
MSWD $\log_e[^{206}Pb^*/^{238}U^{16}O_2] – \log_e[^{238}U^{16}O_2/^{238}U^{16}O]$
$\log_e[^{238}U^{16}O_2/^{238}U]$
$\log_e[^{206}Pb^*/^{238}U^{16}O_2]$
slope of $\log_e[^{206}Pb^*/^{238}U^{16}O_2] – \log_e[^{238}U^{16}O_2/^{238}U]$
y-intercept $\log_e[^{206}Pb^*/^{238}U^{16}O_2] – \log_e[^{238}U^{16}O_2/^{238}U]$
MSWD $\log_e[^{206}Pb^*/^{238}U^{16}O_2] – \log_e[^{238}U^{16}O_2/^{238}U]$

These parameters enable a comprehensive long-term record of calibration parameters obtained during the analysis of mineral standards to be accumulated within a single "Calibration" file. Standard analyses within the Calibration File, uncorrected for common Pb or corrected using either the ^{204}Pb, ^{207}Pb or ^{208}Pb correction methods, may be directly read from the file by CONCH, for grouping, plotting and reporting.

Appendix 4. Constants and abbreviations used

Some key constants used by CONCH are listed below. Standard mineral constants may be viewed and edited using the Runtable dialog.

$\lambda_{U238} = 1.55125 \times 10^{-10} y^{-1}$
$\lambda_{U235} = 9.8485 \times 10^{-10} y^{-1}$
$\lambda_{Th232} = 4.9475 \times 10^{-11} y^{-1}$
Broken Hill common-Pb standard $^{204}Pb/^{206}Pb = 0.0625$
Broken Hill common-Pb standard $^{207}Pb/^{206}Pb = 0.9618$
Broken Hill common-Pb standard $^{208}Pb/^{206}Pb = 2.2285$
CZ3 zircon standard $^{207}Pb^*/^{206}Pb^* = 0.05892$ (Age: 564 Ma)
CZ3 zircon standard $^{206}Pb^*/^{238}U = 0.0914$
CZ3 zircon standard U concentration = 551 ppm
SL13 zircon standard $^{207}Pb^*/^{206}Pb^* = 0.05925$ (Age: 572.2 Ma)
SL13 zircon standard $^{206}Pb^*/^{238}U = 0.09281$
SL13 zircon standard U concentration = 221 ppm
Temora zircon standard $^{207}Pb^*/^{206}Pb^* = 0.055115$ (Age: 416.75 Ma)
Temora zircon standard $^{206}Pb^*/^{238}U = 0.0667839$
Temora zircon standard U concentration = 200 ppm (assumed average value)
91500 zircon standard $^{207}Pb^*/^{206}Pb^* = 0.07488$ (Age: 1065.4 Ma)
91500 zircon standard $^{206}Pb^*/^{238}U = 0.17917$
91500 zircon standard U concentration = 81.2 ppm
Kipawa zircon standard $^{207}Pb^*/^{206}Pb^* = 0.072265$ (Age: 993.4 Ma)
Kipawa zircon standard $^{206}Pb^*/^{238}U = 0.16632$
Kipawa zircon standard U concentration = 250 ppm
MAD monazite standard $^{207}Pb^*/^{206}Pb^* = 0.05767$ (Age: 514 Ma)
MAD monazite standard $^{208}Pb^*/^{206}Pb^* = 19.7177$
MAD monazite standard $^{206}Pb^*/^{238}U = 0.083$
MAD monazite standard U concentration = 1000 ppm (assumed average value)
MAD monazite standard $^{208}Pb^*/^{232}Th = 0.025756$
Khan titanite standard $^{207}Pb^*/^{206}Pb^* = 0.05767$ (Age: 518 Ma)
Khan titanite standard $^{206}Pb^*/^{238}U = 0.083671$
Khan titanite standard $^{208}Pb^*/^{232}Th = 0.02576$
Khan titanite standard U concentration = 700 ppm (assumed average value)
Taz perovskite standard $^{207}Pb^*/^{206}Pb^* = 0.562$ (Age: 463 Ma)
Taz perovskite standard $^{206}Pb^*/^{238}U = 0.0735$
Taz perovskite standard U concentration = 1400 ppm (assumed average value)
Phalaborwa baddeleyite standard $^{207}Pb^*/^{206}Pb^* = 0.12719$ (Age: 2059.5 Ma)
Phalaborwa baddeleyite standard $^{206}Pb^*/^{238}U = 0.3764$
Phalaborwa baddeleyite standard $^{208}Pb^*/^{232}Th = 0.10727$
Phalaborwa baddeleyite standard U concentration = 500 ppm (assumed average value)
M21277 zircon Th-U standard $^{207}Pb^*/^{206}Pb^* = 0.05$ (Age: 2.22 Ma)
M21277 zircon Th-U standard $^{206}Pb^*/^{238}U = 0.0004$
M21277 zircon Th-U standard $^{208}Pb^*/^{232}Th = 0.01$
M21277 zircon Th-U standard U concentration = 900 ppm (assumed average value)

Abbreviations
$^{20x}Pb^*$ = radiogenic ^{20x}Pb
$^{208}Pb^*/^{232}Th$ = (radiogenic ^{208}Pb)/^{232}Th
f206% = 100 × (common ^{206}Pb/total ^{206}Pb)
% concordance = 100 × ($^{206}Pb^*$–^{238}U date)/($^{207}Pb^*/^{206}Pb^*$ date)