CONCH: a versatile Visualbasic software package for the interactive processing of ion-microprobe data

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CONCH is a Visualbasic program developed over the last 8 years to allow flexible interactive processing of ion-microprobe data. It uses algorithms applicable to the processing of ion-microprobe data obtained for a wide range of applications. The development approach was to automate as many repetitive and tedious tasks as possible using sensible default but User-editable parameters, and provide the User with sufficient information to ensure that data quality can be effectively monitored and informed decisions made during data processing. Graphs and tables are generated with limited User intervention, in a consistent style and at publication standard. In this abstract, application of CONCH to zircon/titanite/perovskite, monazite/xenotime and baddeleyite U-Th-Pb, and Th-U disequilibrium dating methods are described.

Input files, run-tables and data editing

SHRIMP output (raw data) files and CONCH-processed data files in three different output formats may be read directly by CONCH. All processing control parameters are assigned default values but these are editable, via the Set-up dialog, 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 data. Alternatively, the mass-station order may be edited using the Run-table dialog, accessed via the Set-up dialog. 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 output) file, with error-checking to notify the user of any values outside the expected range.

Input data for each analysis may be displayed for manual editing on a set of plots of counts (as checkboxes) for each mass station versus analysis time. Alternatively, identification and display only of scans with anomalous counts may be undertaken automatically. For automatic identification of outliers, mass-station counts may be ratioed to secondary beam monitor counts via a checkbox in the Set-up dialog. Software identification of anomalous count values is undertaken using three threshold parameters that are assigned default but editable values in the Set-up dialog. These parameters identify outliers per analysis 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 Background counts 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 plots of counts (plotted as checkboxes) versus analysis time, for assessment by the User. Extensive testing has confirmed that this automated data editing can reliably identify all known instrument-related measurement aberrations, including secondary beam spikes and centring failures (drop-outs). Once editing of the raw data has been completed, the Standards dialog may be summoned.

Identification and editing of session standards

Standard analyses in the input file are identified by the matching of part of the analysis label string with a User-specified standard label string specified in the Set-up dialog. For zircon/titanite/perovskite, monazite/xenotime and Th–U disequilibrium standard analyses, $\log_e {}^{206}Pb/^{238}U$ ratios, corrected for Broken Hill common Pb using the measured ^{204}Pb counts, are plotted in the Standards dialog plot window as checkboxes against $\log_e$ UO/U (or UO_2/UO, depending on that specified in Set-up). Also shown for comparison in the Standards dialog is an uncertainty-weighted regression line of these parameters for the standards and a line with the default slope (usually 2.0 for zircon Pb/U–UO/U). Excess ^{204}Pb (calculated using ^{208}Pb-corrected ^{206}Pb counts) and "hydride" values (based on the ^{208}Pb-corrected $^{207}Pb/^{206}Pb$) with uncertainties for each standard analysis, plus the calculated session means, are displayed in a scrollable list-box next to the calibration plot. Also displayed in editable text-boxes in the Standards dialog are the number of standards, calibration values and slopes, intercepts, uncertainties and MSWD's for uncertainty-weighted Pb/U–UO/U and Th/U–UO/U calibration regression lines. Once editing of the standards is completed, a string corresponding to that of part of the sample labels in the input file may be entered into a Sample Label text-box, to identify analyses to be graphed.

Processing, grouping and plotting of unknowns

Where ^{204}Pb counts on unknowns are comparable with those measured on standards during the analysis session, a common-Pb correction using Broken Hill composition is usually appropriate. CONCH incorporates an option for specifying common-Pb compositions calculated using the method of Cumming and Richards (1975) for analyses of unknowns with ^{204}Pb counts substantially higher than that measured on standards during the analysis session. When ^{204}Pb counts (for monazite and xenotime analyses, corrected for excess ^{204}Pb counts) on unknowns exceed a threshold value (specified in Set-up) times the average ^{204}Pb counts measured on the session standards (also corrected for excess ^{204}Pb counts where appropriate), common-Pb corrections using ^{204}Pb, ^{207}Pb or ^{208}Pb correction methods depending on that specified in Set-up, are made using Cumming and Richards (1975) model compositions.

Analyses may be automatically assigned to $^{207}Pb/^{206}Pb$, $^{206}Pb/^{238}U$, $^{207}Pb/^{235}U$ or $^{208}Pb/^{232}Th$ (depending on that specified in Set-up) age groups and displayed on Wetherill or Tera-Wasserburg diagrams in a group fill colour. CONCH uses an automatic, statistically rigorous analysis grouping algorithm based on the following procedure. Radiogenic $^{207}Pb/^{206}Pb$, Pb*/U or Pb*/Th ratios are weighted according to the inverse square of the individual analytical uncertainty to determine a weighted mean $^{207}Pb/^{206}Pb$ (or Pb*/U or Pb*/Th) ratio for all pooled analyses obtained for the sample. Analyses are then

rejected from the group using two criteria. A chi-square value 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 $^{207}Pb/^{206}Pb$ (or Pb*/U or Pb*/Th) ratio with assigned uncertainty is most different from the weighted mean value will be excluded from the group. In addition, any analysis whose $^{207}Pb/^{206}Pb$ (or Pb*/U or Pb*/Th) ratio is greater than a User-editable threshold value times its standard deviation (typically, a threshold of $\pm 2.5\sigma$ 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, 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 in the Report dialog, and replotted.

Depending on that specified in the Set-up dialog, unknowns can be initially plotted on either Wetherill, Tera-Wasserburg, or Gaussian-summation relative probability density diagrams, with X- and Y-axis ranges and tick intervals automatically calculated using the ranges of the data to be plotted. Axis ranges, labeling, tick intervals and other aspects of the plots may be personalized via Plot Set-up dialogs. The relative probability diagram displays (by default) two probability density curves, one for all (including discordant) analyses, and another for concordant analyses (i.e. $^{206}Pb/^{238}U$ date within uncertainty of $^{207}Pb/^{206}Pb$ date at $\pm 2\sigma$ uncertainty level, or more than a User-specified percentage concordant) only. Switching between any of the plots, assessment and editing of the group assignment and generation of the processed data file, is readily achieved using buttons located on the plot windows and Report dialog. Group labels, giving analysis labels, date and uncertainty, may be added to the diagrams adjacent to analyses using the Summary button.

References

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.