

PbMacDat

At the request of numerous Earthtime II participants, I am posting a simple version of PbMacDat for general use. This Excel Spreadsheet with Macros was conceived of and written by myself at MIT with NSF funding in response to our lab's need for more streamlined data reduction and concordia plotting and the preference for a Macintosh platform. The evolving power of Microsoft Excel with its scriptable and graphical capabilities lends itself well to the multitasking required for large U-Pb datasets. It has been successfully run in Microsoft Excel for Windows, although this has most often demanded some debugging and format alteration. The current version was developed with Excel v.X (Mac OS X).

It is based on the approach of Ludwig (1980) and its main objective is the marriage of the capabilities of PBDAT and ISOPLOT (Ludwig, 1988) for the U-Pb system. It is thus appropriate at this time to thank Ken for his "open-system behavior" with regard to his code. The spreadsheet has been successfully verified against both of Ken's programs for many datasets throughout its development. We consider one of the most powerful aspects of the program its ability to quickly handle real-time "sensitivity tests" by varying input parameters.

It has evolved from its first incarnation (pre-Visual Basic) to the present Visual Basic version with much effort from Drew Coleman for the initial re-coding and since that time has evolved in that format with continued tweaking and inputs from Drew, myself, and Mark Schmitz. We sincerely hope users will adapt this program to their own needs using their own Visual Basic for Excel expertise. The aforementioned have all done so, hence the need to strip it back to a more generic version. For anyone using this often, it is almost a requirement to have someone in your group become familiar with the code, not a trivial task but a great learning experience for budding geochronologists. Furthermore, none of the original scripters want to quit our day jobs to become full-time troubleshooters. However, we recognize the probable need to act as facilitators in the early going.

This version of PbMacDat comes with a sample dataset for instructional purposes. Before reducing your own data, you will need to fill in all pertinent parameters in the Lab Constants worksheet (see below). Following is a demo exercise to familiarize you with the main features of PbMacDat. Before beginning play, make a back-up copy of PbMacDat.¹ If the file downloaded with any additions to the filename, it will crash. **Be certain the file is named PbMacDat (no spaces, no .xls suffix) before opening.**

¹ PbMacDat will crash if run under a different filename. i.e. "PB MacDat-copy" will not be recognized by many macros. Nor will PbMacDat.xls.

- 1) File opens in the Raw Data worksheet². There is an opening message which disappears when you click on it. There are seven data points entered in the upper raw data portion of the sheet. The worksheet will accommodate up to 100 analyses. These inputs include fraction identification, sample and spike weights, and raw ratios from mass spec runs with associated percent error at 1 sigma. The last two inputs are for collector configuration which determines the fractionation applied (D = single Daly, F = Faraday-Daly combined, C = custom), and spike used. There are buttons at the top that facilitate the entry of these. F and D's have already been entered in this example. Select a cell in one of the data-filled columns and click on the {SPIKE 1} button. This enters the spike name in the appropriate cell for that column. This not only expedites entry, but also ensures proper spike identification from the Lab Constants sheet (more on that later).

- 2) To reduce a data column once it is filled, simple select any cell within that column and click {REDUCE DATA}. This action copies the raw data to the Reduce Data sheet where the result is immediately displayed. A number of actions can be taken from this sheet and are summarized below.
 - a. Cell Entries
 - i. Any values may be changed in the raw data column, and below that, inputs may be changed for blank estimate, initial Pb correction method (SK = Stacey Kramers, CR = Cumming Richards, C = custom entry in the subsequent columns), and custom fractionation (in %/amu). The latter is activated by placing a "C" in place of F(araday-daly) or D(aly), above.
 - ii. NOTE: These are the only cells that should be changed manually. In general, blocks of cells surrounded by a double border should not be touched.
 - b. Buttons (from top to bottom)
 - i. Clicking the calculator button at top to run the calculation must follow any manual changes to the raw data.
 - ii. The data output at the right of screen can be printed with the Printer button.
 - iii. Any combination of raw and reduced data can be dumped back to the Raw Data worksheet with the next three buttons. Fractions with the same names will be overwritten on a raw dump. Changing the Fraction ID will create a new raw column.
 - iv. {Activate Data File} button will flip you back to Raw Data sheet (conversely, {Go To Reduce} will flip you the other way).
 - v. Buttons at lower left will be discussed later.

- 3) Dump Reduced Data: this will begin to fill up the reduced data table in the Raw Data sheet. This table can be filled up point by point or, by clicking the

² Depending on monitor size and resolution, it may be desirable to resize the field of view using the Zoom command (View-Zoom). The field of view is also be enhanced by using Full Screen option.

{REDUCE ALL POINTS} button, en masse. Once the table is full of reduced data, various actions can be taken. Note that the “symbol” column acts as a flag for selecting subsets of data, and thus is the only interactive column in the lower table (flag symbol is “a”). Reduced data button array (l to r):

- a. Data can be sorted by age (207/235) or fraction name.
 - b. To delete a line of reduced data, select a cell in that line and click “Clear Line” button
 - c. “Clear Table” button does just that.
 - d. “Print Short Table” prints out a publication-style table.
 - e. “Print Long Table” prints out a table containing reduced as well as raw data.
 - f. “York Fit” fits a linear regression to all fractions containing an “a” in the “symbol” column. As the days of discordance fade to history, this feature may begin to feel neglected.
 - g. “Weighted Mean” and “View Statistics” show statistical results for all fractions containing an “a” in the “symbol” column.
 - h. Green Concordia button opens the Concordia Plot worksheet (more on that below).
 - i. If reduced data is entered manually into the reduced table, “Make Ellipse(s)” will generate ellipses on Concordia. This is useful for entering U-Pb data from the literature, for example. Required columns for such a calculation include U-Pb ratios and errors and corr. coef.
 - j. “radcom >20” flags only those data points with a radiogenic/common Pb ratio greater than 20 and acts as a first pass filter.
- 4) Concordia Plot worksheet will display reduced data on a conventional Concordia diagram or a Tera-Wasserburg plot. Another array of buttons are at your disposal:
- a. {Raw Data} is simply a worksheet toggle.
 - b. {Ellipse Centers} and {Ellipse Labels} are toggles for plotting center points and labels. These will only plot for data flagged with an “a” in the reduced data table, and the labels will only appear when the centers are displayed.
 - c. The next three buttons are for resizing the axes. {Initialize Axes} will redraw Concordia to show all data points, {Min/Max AGE} and {Min/Max X-Y} will prompt dialog boxes for user input age range, and X-Y ranges, respectively. Initialize now to see all points.
 - d. {Yorkfit} will regress all flagged data points and plot the discordia, intercept ages and errors, and MSWD. When clicked, you are prompted for an estimate of the upper intercept age (in Ma). For a poor fit, you will be prompted to consider using a model 2 regression. To remove regression, toggle {Yorkfit On/Off}. {Error Envelope On/Off} and {View Statistics} are self-explanatory.
 - e. {View Summary} shows a printable and savable summary sheet containing concordia and reduced data table, with space for an imported jpeg.
 - f. {Tera-Wasserburg} shows alternative display of data.

- 5) Archiving Data: All raw and reduced data can be easily archived as a separate file for later upload into Pb MacDat. It is initiated with {Save as Archive} button at top of Raw Data worksheet. It helps at this point to know the directory string (e.g. Macintosh HD:Users:Me:Desktop:UpbFiles) to which you want the file saved. It will be saved there with a filename corresponding to the Sample ID specified at upper left of Raw Data worksheet.
- 6) Lab Constants is a hidden worksheet that can be accessed via a button in lower left of Reduce Data worksheet. It corresponds with the LabData FILES of Ludwig (1988). It is password protected (password = zircon) and may be unprotected via the Tools menu. If you wish to maintain its protection you will need to re-protect when finished, and rehide via the Format Menu (Format:Sheet:Hide). The four labeled spike columns (SPIKE 1 thru 4) are the only columns supported by rapid entry buttons at the top of the Raw Data worksheet. These generic names can be replaced here in Lab Constants (just type the new name over the existing name) and on the buttons themselves by control-clicking the button and replacing the text. Note that SPIKE 1 and 2 are triple spikes and 3 and 4 are double spikes. More spikes can be entered and used, but they will not have the convenience of button-activated cell entry without coding for new buttons. For appropriate entries in Lab Constants, the user is referred to Ludwig, 1988a.
- 7) Uploading archived data: When data is archived it is saved to a separate workbook with an embedded activation button for sending data back to Pb MacDat. The only proviso is that Pb MacDat must already be open.
- 8) Happy Crunching.