Changes to the beta version of PhreePlot

23 May 2011   beta

- A second colour can be added to the backgroundColor keyword to denote the page colour. The backgroundColor of custom plots was previously overplotting the plotted lines - this bug has now been fixed.

- A new type of plot, a 2D 'contour' plot, has been added. See the documentation for details.

- Tags can now be added anywhere in an input file including in the PhreePlot section (before the 'Chemistry' keyword). Previously tags in this section were limited to post-calculation keywords such as plotTitle and extraText.

20 December 2010   beta

- The plotting of symbols and lines has been enhanced. You can now define your own line colours, line widths (dashed or not), point (symbol) colours and point sizes (and for 'filled' symbols, their rim colour and rim width) for individual datasets. This has been done by extending lineColor, pointColor etc to take a list instead of a single value. This has necessarily changed the logic of the auto-generated colour sequence for multiple lines slightly since rather than continuing the auto colour sequence after lineColor(1) (as before), named colours are simply promoted to the top of the autocolour sequence and then colours picked from this modified list one by one. Each feature (line, point, rim etc), including their 2y counterparts, has its own independent colour sequence. This means that there is now usually a 1:1 positional relationship between parameters in the various lists, say, between a 'lines' list and the corresponding 'lineColor' and 'lineWidth' lists making it easier to specify colours in complex situations. New keywords pointType, rimColor and rimFactor have been added.

- Properties for datasets plotted on the 2y axis now have their own keywords to match those of the main y axis, viz. lineColor2y, lineWidth2y, pointColor2y, pointSize2y, rimColor2y, rimFactor2y.

- Some of these features are illustrated in the demo\symbols\plotsymbols plot below.
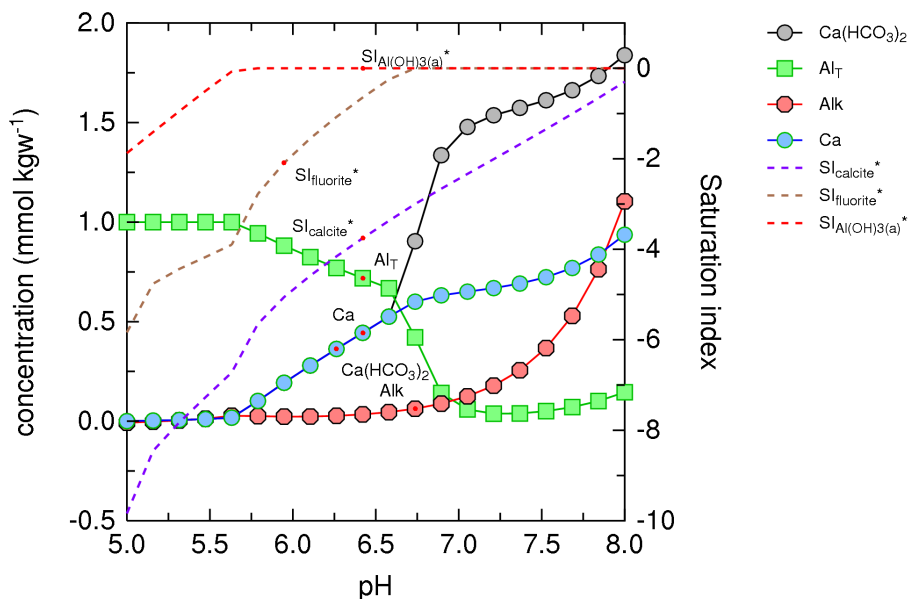
- additional optional parameters have been added to the extraSymbolsLines file format used for drawing customised points and lines to enable the symbol type, rim colour and rim factor to be specified.

- Black is no longer the first auto line colour chosen for lines and symbols but the last (to make it easier to get a full set of auto-coloured lines excluding black).

- In general, colours in the various input lists (lineColor, pointColor, ...) are simply appended to the front of their respective auto-colour lists. Other properties, such as line widths and point sizes, are also selected from the corresponding input lists (lineWidth, pointSize, ...). However, when these run out, the input list is simply recycled.

- Unfortunately these changes mean that some auto-colours will be different from those generated in earlier versions of PhreePlot. This is most likely to occur when all colours are auto selected or when subsets of data are being plotted (when one column of data contains one or more blank lines indicating subsets of data). Normally 'changeColor T' will ensure a varied set of colours or an explicit 'lineColor' setting may be able to be used to set the colours. It is always possible to get your old colours either by modifying the ppi script or by editing and using the line colour dictionary.

- Since lineWidth is now a list, the second optional lineWidth parameter giving the dash frequency has been given its own keyword, dashesPerInch, so that lineWidth only contains line widths.

- A value of 0 for pxminor, pyminor or p2yminor turns off the plotting of the respective minor ticks.

- The third parameter on title2y which indicates the character string appended to labels referring to the 2y axis can now be a character string of up to 40 characters rather than just a single character (e.g. making ⁺ possible).

- The automatically generated <date> tag has been renamed <timedate> to more accurately reflect what it is.

- 'Carry' variables in predominance plots now get written to the track file as well as the out file.

- minor improvement to the ht1 algorithm to avoid a quite rare problem when an intersection was very close to an edge.

- The recovery mode (calculationMethod 3) of a 'grids' plot has been improved so that it should now be better able to recover from crashes.

- 'Domain tags' can be used to skip the speciation calculations in specified (i.e. 'problematic') parts of a predominance diagram by clipping the calculation domain - this should speed up some calculations.

- Changed the order of precedence when plot labels are auto selected but defined in more than one place: now the precedence is: the 'labels' keyword, then the loop file, then the data file column heading. Where several subsets of data are plotted, the latter two approaches append a subset description, "_n" to the label name. Labels defined with the 'labels' keyword are always used *as is* without any such adornment.

- the 'extraOut' keyword has been renamed 'extradat' to better reflect what it does. The old keyword still works as an alias.

- redefined the SURFACE_MASTER_SPECIES of the cdmusic_hiemstra.dat database to dummy uncharged species in order to avoid the addition or removal of charge when a surface is added or removed. The convergence criterion has also been increased (i.e. made less onerous) in the cdmusic_hiemstra.dat file to facilitate convergence. Thanks to Tony Appelo for this.

- Updated to IPhreeqc-2.17.5-4962. This has solved some non-convergence problems.

- Other minor changes to the output and some bug fixes.

26 June 2010   beta

- A bug was introduced in the last update which prevented the 'grids' example from plotting. Fixed.

- the include file 'minstab1.inc' which is used for preparing mineral stability diagrams sorted the minerals in ascending order of abundance rather than descending. This meant that the wrong mineral was promoted as the most abundant when two or more minerals were present simultaneously. Fixed in the minstab1.inc script.

- tabs, including leading tabs, are now always treated as significant separators in the datafiles used for 'fit' and 'simulation' calculations whenever the separator is set as the generic separator ("" for blank, tab or comma).

- if there is a failure in speciation during a simulation such that the expected selected output is not produced, a row of data is now written to the 'pts' file but without any selected output (since there is none). This keeps the selected output in sync with the other sample data that are written to the 'pts' file. However, as before, no lines of data are written to the 'out' file for these failed cases.

- 'speciesvsph.inc' and related files now filter out gas, '...(g) ', species before appending '(s)' to any pure phase species names.

- the pp.log file now contains two entries per run, one for starting and one for finishing. This ensures that there is always an entry even for runs that crash mid-run.

- now allows an unlimited total length of polygon edges in 'grid' plots.

- changed the way that PhreePlot determines the full path of the input file to make it more compatible with the WINE Windows 'emulator' for Linux.

- an updated version of PHREEQC (2.17.0.4466) has been incorporated.

8 March 2010   beta

- the line colour dictionary is now always updated for custom-style plots even when no labels are drawn. This ensures that the colours at least are always re-written to the file.

- some of the linecolor.dat colour dictionary files in the distribution were old-format files without the points colours - these have been updated to the new style.

- some fields could be left uninitialized when a variable number of columns were written to the selected output file during 'fit' or 'simulate'. This could result in garbage being written to the log and pts files.

- temporary data is now written to disc rather than to memory during 'fit' and 'simulate' enabling larger problems to be run.

2 March 2010   beta

- an updated version of PHREEQC (2.17.0.4137) and its databases has been incorporated.

- in the log file, the range of pre-loop simulations was reported as ending on the last simulation in the block rather than the last pre-loop simulation. Fixed.

- spaces in the input file and directory names were causing problems when attempting

to expand to the full path (a 'File not found' message was written to the console). Not fatal, but irritating. Fixed.

- now checks more carefully for a valid data separator following the 'datafile' keyword. The presence of a single (invisible) tab was causing problems.

- the progress ('p') plot for predominance diagrams went AWOL on the 4 November 2009 update and has been reinstated. The plotFrequency keyword also now works.

- the last update also caused the 'Resimplify and replot' option (calculationMethod = 3) for 'grid' plots to recalculate rather than reading from the existing track file. Fixed.

- added 'total dissolved concentration' to the include files, speciesvsph.inc and logspeciesvsph.inc, which are used to generate 'species' plots. The new files are speciesvspht.inc and logspeciesvspht.inc, respectively. Useful for preparing species plots when adsorption or mineral precipitation is taking place.

- the xaxisisphtol keyword has been removed.

- the initialValue keyword has been added - any numeric tags that are undefined at evaluation time are set to the initialValue (default = UNDEFINED, i.e. -99999).

- added the system tag <nexecute> which is automatically filled with the number of times that PHREEQC has been called.

- the JAEA and NEA PHREEQC-format databases (011213c2.tdb Rev. 2, http://migrationdb.jaea.go.jp/english.html and 050000c0.tdb, Rev. 0, http://migrationdb.jaea.go.jp/tdb_e/d_page_e/d_0500_e.html), the stable isotope (H, O, C) database (iso.dat) and the Specific Interaction Theory (SIT) activity coefficient model database (sit.dat), the latter two both distributed with PHREEQC, have been added to this distribution. Tables showing which elements are defined in which databases plus links to the sources have been added to the Guide (see Appendix 2).

- Hiemstra et al.'s CD-MUSIC model for U adsorption by ferrihydrite is now included in the demos - see the UFhy directory. The new themo data associated with this model have been added to cdmusic_hiemstra.dat in the \system directory. The other CD-MUSIC examples have been updated to use this database.

- input errors caught by PHREEQC in the Chemistry section are treated as fatal even for predominance plots with debug=0 when they are found in pre-loop simulations.

- minor updates to the Guide.

15 December 2009   beta

- minor changes to output.

9 December 2009   beta

- corrected a bug introduced in the last update in which the internal treatment of batch files occasionally caused the input file to be deleted.

7 December 2009   beta

- added a new plotType 'grids' which is the same as 'grid' except that it calculates predominance diagrams for multiple 'main species' in one pass through the speciation calculations. This uses the 'grids.inc' include file. This should be faster than 'grid' for preparing predominance plots for several elements for the same 'system' especially for complex chemical systems where the speciation calculations are relatively slow.

- corrected a bug in which the estimated pe of unmeasured points in a 'grid' plot were sometimes wrong. This affected the conversion of grid plots between 'native' and pe-based scales and was most noticeable with low resolution grids.

- the 'font' setting was not accepting many of the font family names. It is now. Also revised fonts.dat.

- if tabs alone are chosen as data separators in a data file, then a blank string before the first tab (leading blank) is now treated as significant whereas previously it was skipped over.

- when reading in a data file, completely blank fields in a numeric column are no longer treated as errors but are filled with the missingValue setting.

- PUNCHED'ed data in 'simulate' runs is now correctly written to the pts and log files.

- autoscaling now takes into account any clipping of data.

- during 'fit' and 'simulate', instead of stopping immediately when there has been a lack of convergence in PHREEQC, PhreePlot will now only stop after having completed calculations for the complete set of data.

4 November 2009   beta

- revision of how PhreePlot deals with complex, multi-simulation PHREEQC input files. This is centred around the division between 'pre-loop' (initialization) and 'main loop' simulations. Now has a more flexible structure especially especially for fitting which includes the ability to define a different block of simulations with blockRangeColumn (fomerly fitSimulationColumnNumber)and mainLoopColumn. 'mainLoop' is the new primary keyword (formerly 'loopSimulationStartNumber'). Aliases still valid.

- re the above, an important change is that 'selectedOutputLines' now refers to PHREEQC simulation numbers directly not 'run' numbers. This should make it easier to specify.

- because of the above, the ison, isopp and kineticsSifit examples need an extra line ('mainLoop...' or 'selectedOutPutLines...) to work properly. See the new files.

- there is better logging of the simulations being run in the log file so that you can better see what is going on (especially with debug = 2).

- improved autoscaling when the 2y axis is being used.

- tags can now be included in the list of 'points' and 'lines' variables.

- tags created with numericTags are now initialized with the value 0.0 rather than the undefined value (-99999.0). This permits, e.g. <sum> = <sum>+<val>.

- added the rand(iseed) and nrand(iseed) functions to the tag expression parser. These generate a pseudo random number from the uniform (0,1) and normal (mean=0, standard deviation = 1) distributions, respectively.

- minor changes to the labelling of custom and predominance plots.

- redundant headers and blank lines have been removed from the 'out' file of species plots.

- lines/points were sometimes omitted from a custom plot when some other variable was plotted on both the y and 2y axes.

- legend (key) entries for custom plots are now sorted so that all points are plotted first, then all lines.

- the '*' appended to 2y labels in custom plots was preventing them from being interpreted as valid PHREEQC formulae - e.g. they were not being sub/superscripted. They are now.

- edited the input and documentation files to get a consistent use of the primary keywords which had gradually diverged with the changes.

- added debug = 99 option. If this is set, e.g. in pp.set, then all keywords read from input files from thence forth will be checked to see if they are primary keywords or aliases. A list of the aliases used and their primary keywords will then be given.

- it was originally planned to release PhreePlot 1.0 about now but there is still quite a lot to do so it looks as if it will remain in beta testing until sometime during 2010. During this phase, I'll release fairly regular updates. Re-installing PhreePlot with the latest version does not replace or delete any of the files that you have generated just the ones that PhreePlot put there in the first place.

16 September 2009   beta

- two examples of animation added to the web site.

- additional variables can now be added to a species plot with lines, points etc.

- during plotting after fitting, the selected output was not being written to the points file when a blank line was written to the selected output. Corrected.

14 September 2009   beta

- corrected a bug when a multiple-simulation range was specified in the fitSimulationColumn of fit data files.

- improved diagnostics when there was incorrect input during fitting.

- improved documentation and demos, especially for fitting.

9 September 2009   beta

- added two new options for the choice of fitting algorithm (fitMethod = 'newuoa' and 'bobyqa'), both by MJD Powell. These augment the existing 'nlls' fitMethod, also by Powell. See the Guide for the setup which is broadly similar. 'bobyqa' includes simple constraints (lower and upper limits).

- the 'digits' option controlling the number of digits printed when a tag value was used in an extraText file was not implemented properly (the default value of -3 was always used).

- the dependentVariableColumnIn and dependentVariableColumnOut keywords used in the demo examples have been replaced by their main keywords, dependentVariableColumnObs and dependentVariableColumnCalc, respectively. This ties in with their use in the Guide. The corresponding 'in/out' keywords were aliases and so worked anyway.

- the line colour dictionary was not being written when there were no labels to plot (but when some lines and/or points were plotted).

- the primary keyword for loopSimulationStartNumber was changed to its alias simulationStartNumber.

- re-revised code for auto choosing of pxdec, pydec.

14 August 2009   beta

- the updated CD-MUSIC database (\system\cdmusichiemstraJuly2009.dat) and ecosat.dat files were mistakenly omitted from the 6 August release.

- improved autoscaling (pxdec, pydec).

- added an optional second parameter to minimumYValueForPlotting which applies to the 2y axis.

- the number of data points reported to have been read from an outfile was not reset properly when multiple files were read. The data were actually read properly though.

- better diagnostics given when an unrecognised outfile column name is given for plottting. An unrecognised column name will now result in a fatal error rather than just being ignored.

- the reformatted text at the end of the log file was not reformatting the extraOut line(s) properly.

- added a file with the missing data (pHb) for the Hfo_titration.ppi demo.

6 August 2009 beta

- improved autoscaling for custom plots.

- extra spaces have been introduced on the screen output showing the progress during the calculation of predominance diagrams to improve legibility.

- 'Plotting_error' exit sometimes gave an overflow writing to pp.log file.

- If XMIN is not less than XMAX, now always produces a fatal error; ibid YMIN, YMAX.

- removed the CO2(g) constraint from the wateq4f example series of predominance plots. Also removed possible adsorption by Hfo since Fe(OH)3(a) was never the most stable Fe mineral species and so adsorption to Hfo was never a possibility. Added the ppi files used to generate these diagrams to the demo directory.

- CD-MUSIC database for goethite ('cdmusichiemstra.inc') updated. File moved to the \system directory as 'cdmusichiemstraJuly2009.dat'.

- some new CD-MUSIC examples added to the As-cd-music demo directory. Also added these examples to the web site.

- label for 2y-axis sometimes had multiple '*' (the 2y indicator) appended.

- a line was sometimes incorrectly drawn after a line break in the extrasymbolslines file.

- some of the automatically-generated plot tags, <pxmin> etc., were incorrectly listed in the log file as being used when they were not.

- <p2ymin> and <p2ymax> were added to the list of tags that are automatically generated.

- lines2y was not being written to the reformatted input file.

- minimumyvalueforplotting is now applied after clipping to the plotting domain.

- posted data values got out of sync when data was clipped to the plotting domain.

- web site: PhreePlot tags in the html code were not being interpreted as text when viewing the code used for generating the plots. This caused some of the code following such tags to be missing or incorrectly displayed.

- Ghostscript has recently been updated to Version 8.70 but I had problems with the

epsi conversion with this new version so have kept the default pdfMaker setting at 8.64. If you install a later version, remember to change the pdfMaker setting in pp.set to make sure it matches what you actually have installed and update your bin and lib paths too.

- PhreePlot guide: various corrections and minor changes.

14 March 2009   beta

- up and running

- beta release www.phreeplot.org