

Changes to PhreePlot

2024

6 September 2024

Version 1

- Added automatic generation of <nIter> tag to give the number of function evaluations after a fit.
- Now includes the THEREDA database for high ionic strength media (Pitzer model).
- Repeat factors can now be used for all keyword values in non-quoted text in the PhreePlot section of the input file, e.g. `lineColor 7*red4 2*blue`. Use quoted text to avoid conversion especially in `numericTags`.
- Improved treatment of multiple selected output blocks.
- `pageOrientation` can now be specified as 'portrait' (old '0') or 'landscape' (old '1').
- `svg` image file export activated – makes use of a user-supplied external app to produce image.
- A new system tag, <contourZvariable>, has been added to give the current value of the `contourZvariable`.
- `extraText/text` blocks – there is now no vertical alignment setting.
- for fitting with `bobyqa`, `newuoa` and `cobyla`, now `RHOBEG` = 0.1 x `fitMaxStepSize` (as recommended). `RHOEND` = `fitConvergenceCriterion` as before.
- Minor improvements to text positioning especially 'auto' positioning.
- `LLNL_AQUEOUS_MODEL_PARAMETERS` no longer requires 25C or less minimum temperature.
- A new setting, `axisNumberFormat`, has been introduced to control the format of axis numbering with very small or large numbers, namely, whether to use 'native' numbers like, 0.00001 or use an 'exponential' format ('exp') which rescales the numbers by dividing by a factor, e.g. "/10⁻⁵". The default, 'auto', attempts to make a sensible choice.
- Updated to `iPhreeqc/PhreeqcRM 3.8.2-16969`:
<https://github.com/usgs-coupled/iphreeqc> (Win32)
<https://github.com/usgs-coupled/phreeqcrm> (x64)
- Fixed known bugs and minor improvements.

2023

24 February 2023

Version 1

- Fixed bug for multiline legend titles in contour plots – some overwriting `cos y` not

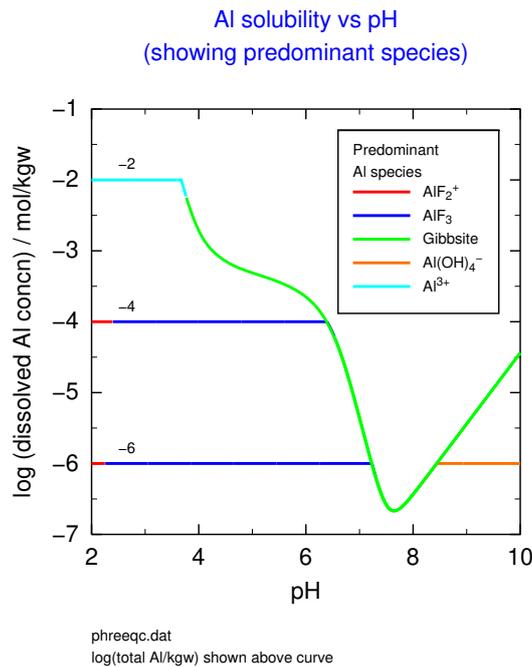
calculated correctly

15 February 2023

Version 1

Mostly minor changes but the first one provides a new and interesting plot and the second one can be useful, e.g. when high pH/CO₂ causes failure.

- The dataSeparators break="`<column_name>`" now also breaks on a character column when the value changes. Previously it only worked for a change in the sign of the slope for numeric columns. This makes it relatively easy to change the colour of a line according to some specified condition. One application is to produce a 1D predominance plot as shown below.



The plot shows the solubility of a simple Al-F-S-C solution with varying pH and total Al concentration (10e-6, 10e-4 and 10e-2 mol/kgw). The colours of the lines reflect the dominant Al species present (see `\demo\Alvsphpredom` for the example and the Guide for details).

- If a speciation fails generating a custom plot, this formerly caused the run to abort but now the calculations will normally continue to produce a plot with the available data.
- 'SelectedOutPutFile' now has an 'append' option.
- 'points' has an 'auto' option which means that all lines plotted will have their points plotted too.
- PUNCH'ing `eoI$` previously assumed this was a character variable and so enclosed it in quotes. It now does not include the quotes.
- The default background colour for legends was 'nd' (i.e. transparent); it is now the same as the colour of the plot area or 'white' by default. This makes more sense when a grid

is also plotted.

- `backgroundColor(3)` now also applies to text added with `text/extraText`.
- `svg` keyword parameters have been changed slightly. Actually you can now use this keyword to run any sort of external post-processing program. See the Guide.

28 January 2023

Version 1

- Moving a legend with `'text/extraText'` did not move the title. Does now.
- Add `\Ureview` to `\demo` directory. These are scripts used to do some of the PHREEQC calculations found in our U review paper (<https://www.sciencedirect.com/science/article/pii/S0883292722003389>)
- Added a link on `phreeplot.org` to a new app (`lsp.exe`) which analyses PHREEQC-format database files.

2022

11 October 2022

Version 1

- New keyword, `'axisNumberFormat'`, which determines whether the `'exponential'` format is used for axis numbering (`'auto'` = if necessary; `'native'` = definitely not).
- New keyword, `prefix`, added to redirect all output files to a specified directory.
- An additional optional parameter has been added to the `ps`, `png`, `pdf`, `jpg`, `eps`, `svg` flags to enable the filename to be set explicitly rather than being auto-generated.
- Corrected bugs related to use of nudges and a `nudgefile` and the use of quotes in the header of an `'outfile'` which sometimes prevented replotting.
- Corrected bug for the auto conversion of the `yscale` from `'native'` to `'mV'` scale in contour plots (it divided the calculated `Eh` by 1000 rather than multiplied it by 1000!).
- Improved auto positioning of text.
- Corrected the y-axis title position when the exponential format was invoked.
- Parsing the track file for replotting grid plots failed because of a failure to read species names containing spaces properly. This has been corrected by adding quotes in the track file (as previously).
- Empty `trk` file written for custom plots – now nothing is written
- blank input lines with tabs were not being skipped and so could upset the number of simulations identified if at end.
- added further adjustments to legend box position.

3 February 2022

Version 1

- Missing dll's can arise from time to time and prevent PhreePlot from running properly. The installation notes on the website have been updated to provide better guidance about how to overcome such problems. A subset of possible missing dll's available in the missing dlls-***.zip file distributed with PhreePlot has been extended with an online version – see the link on our installation notes page. Please report any problems.

24 January 2022

Version 1

- Updated to Phreeqc-3.7.3-15968.
- A trial version of PhreePlot for Linux and Mac operating systems has been developed by Marino V. Zuccolini. See www.phreeplot.org for details.
- Updated the capabilities of fitting: can vary the objective function between least squares, L2-norm, and the minimum sum of absolute deviations, L1-norm; can fix the same target objective function for all fitting methods (see the objectiveFunction keyword); now get approximate standard errors and correlation matrix for all fitting methods not just 'nlls'.
- Added another background colour for the background to text labels in plots. See backgroundColor keyword.
- More flexible character tags including concatenation and trailing blanks.
- Maximum length of Postscript text strings increased from 200 to 400 characters.
- Improved auto label placement.
- Restructuring and minor fixes.

23 July 2021

Version 1

- Added a new keyword loopVal which is an alternative way of defining a discrete set of loop values, not necessarily equally spaced.
- Colours can now be defined in rgb format as well as in the Cohort notation (red4 etc).

4 March 2021

Version 1

- The checkForUpdate has not been working since the website was upgraded to https (on 8th February). This has been fixed by adding a new wget.exe.

8 February 2021

Version 1

- Fixed y auto-scaling issue on multiple plots.
- Allowed for gases to be specified as H2,g rather than H2(g) etc.

4 February 2021

Version 1

- A couple of bug fixes.

7 January 2021

Version 1

- There have been a series of issues with installing and running PhreePlot in recent weeks

which I have tried to resolve. Please let me know if you are having problems (david@phreeplot.org).

2020

31 December 2020

Version 1

- The previous release (22 December) was linked to the wrong runtime library (dynamic rather than static Windows library) and gave inconsistent results especially for system calls including calls to Ghostscript. Fixed.
- There was also a bug in running some system calls, notably for the Ghostscript file conversions. Fixed.

22 December 2020

Version 1

- Fixed an issue with auto legend placement in multi-file custom plots (now reset for each plot).
- Installation: if pdfMaker was not explicitly set to the path for the Ghostscript executable (the default), PhreePlot complained about it and sometimes gave the message "Ghostscript executable not found" if a file conversion was wanted.
- A separate x64 installer has been included on the website for those who do not have access to administrator rights for installation. Please report any problems.
- Changed the way pe is interpolated for grid plots. Now exclude any readings where $pe + pH < 0$, i.e water has decomposed. In practice, this makes little difference to the final plots.
- The archaic epsi file format is no longer supported by Ghostscript and has been removed from PhreePlot. The eps format can also be unreliable and is no longer supported by Word and some other applications. It is also best avoided. Use png, pdf or jpg and either clip outside or within the application.
- Modified the *.inc files used to prepare predominance diagrams to skip over very small concentrations ($<1e-12$) and thus avoid sometimes spurious data.

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4 May 2020

Version 1

- Update Phreeqc to 3.6.2-15100.
- Inline versions of two keywords used for adding text, symbols and lines to plots have been added. The inline versions are alternatives to the extraText and extraSymbolsLines keywords which read settings from a file. The inline versions have a similar format but avoid having to add an extra file.

- The nudgeFile keyword also has a new and revised inline version, nudge. This has been revised so that multiple similar labels on a plot can now be distinguished. This has changed the format slightly but all the old functionality has been retained. Nudging of labels now applies to all types of plots and is the easiest way of refining the position of labels. See the Guide for details.
- The yscale keyword now also applies to contour plots. This enables conversion of pH-O2(g) plots to pH-Eh, pH-pe etc plots providing the other critical parameters such as pe and temperature are also exported in the USER_PUNCH keyword block.
- legendBox now also reads the x,y coordinates so as to place the legend anywhere on the plot.
- Support for the ai output format has been dropped. Use ps, eps or pdf instead.
- Bug fixes and minor feature changes.

2019

13 May 2019

Version 1

- Fixed two bugs – one affected label placement in predominance plots when some fields were not drawn; the other corrected the late update of the <phreeqc_status_0> tag.

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1 May 2019

Version 1

- Updated to Phreeqc 3.5.0-14000.
- Labelling - useLineColorDictionary 2 was not plotting the labels on custom plots and some fields were sometimes not being labelled in grid plots Fixed.
- The labels “O2(g)...” and “H2(g)...” have been given some special treatment in order to make them better-placed on Eh-pH plots (they are automatically rotated and are printed even when their polygon boundaries are not).
- The ‘.lab’ file produced during predominance plots now includes a column with the position of the labels in the same units as the plot scale (e.g. Eh). This file can now be more easily edited and PhreePlot rerun (plotMethod = 2) to reposition the labels.
- Contouring – can specify fixed (e.g. _3) or exponential (e.g. \$3) format and significant figures using the ‘contour’ option as well as with the contourLabelFigs keyword. The yscale keyword can also be used to change the y-scale as in predominance plots providing that the pe and for Eh/mV, temperature, TC, are also PUNCH’ed and given the column names ‘pe’ and ‘TC’, respectively.
- Not specifying a valid contourZvariable for a contour plot is now an error (rather than taking the first variable in the outfile).
- A new keyword LegendTextColor controls the colour of legend text.
- GSview does not accept %PhreePlot Path% as the location of the GS dll so in GSview’s

Options | Advanced Configuration, change to the appropriate folder explicitly, e.g. C:\Program Files\PhreePlot\gsdll64.dll.

- The default format for the plotting of small tag values (less than $\text{abs}(1e-4)$) is now exponential format rather than floating point format.
- The default lineColor/pointColor has been changed from 'black' to 'auto'. This often means that the first color in custom plots is 'red' rather than 'black'. This now gives lines the same auto sequence as points.
- Parsing of fit datafiles improved.
- Installer better able to deal with overlapping Win32 and x64 installations.
- Updated the embedded version of Ghostscript to 9.26RC1 (we found problems with an incorrect bounding box during eps conversion in 9.27).