

# Changes to PhreePlot

## 2022

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](http://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](mailto: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-O<sub>2</sub>(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 “O<sub>2</sub>(g)...” and “H<sub>2</sub>(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  $\text{abs}(1\text{e-}4)$ ) 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).