

Changes to PhreePlot

2016

24 December 2016

Version 1

- There was sometimes a string overflow that caused a crash in predominance plots. Fixed.
- 'yscale' can now be set to 'Eh' etc in contour plots to effect the transformation of the y scale under rather special conditions, just as for predominance plots.
- the names of the 'nudge' files for the last minute moving/rotating of labels were previously fixed as dlabels.set and labels.set, but are now set by a new keyword, nudgeLabelsFile.
- 'auto' for the plot number in a nudge file was only applied to the first plot. Fixed for all plots.
- Updated to [Phreeqc_3.3.9_11951](#).

10 November 2016

Version 1

- If the gridLines setting was short (<6), the values were not being recycled for the 2y axes.

1 November 2016

Version 1

- No new features added.
- Fixed a regression. The fill colour dictionary for predominance plots was not being updated properly when multiple plots were created.
- Updated to [Phreeqc_3.3.8_11728](#).

18 July 2016

Version 1

- Multiple plots can now be combined with the main plot using multiple instances of the 'overlay' keyword. This makes combining plots to make quite complex layouts possible.
- Implemented the recent changes to multiple SELECTED_OUTPUT/USER_PUNCH in Phreeqc. SelectedOutputLines is now a single value (not a list as before) that specifies the number of lines of selected output sent to the 'out' file and therefore potentially subsequently used for plotting. The number of lines are counted from the bottom of the selected output. The selected output block used will always be the block with the highest user number, n, i.e. from SELECTED_OUTPUT n/USER_PUNCH n (default = 1). This doesn't have to be the last definition in execution order and so can be used to direct output from an earlier simulation to the 'out' file.
- The arguments for the selectedOutputFile keyword have also changed – it now has just one argument, the logical switch which determines whether the selected output file(s) are written to disc or not (previously this was the second optional argument). The selectedOutput filename (formerly the first argument) is no longer used or allowed.
- By default, the bounding box for eps files is now calculated with the Ghostscript bbox device driver.

- Some internal restructuring including a new species dictionary.
- Negative adjustments to the position of the legend box were not accepted; they are now.
- The 'lm' fitting method was using a fixed convergence criterion of 1e-6 rather than the criterion set by fitConvergenceCriterion. Fixed.

15 February 2016

- Added the latest set of PHREEQC database files missing from the 11 February update.

11 February 2016

Version 1

- Blank field names are now allowed in predominance plots.
- Removed the limitation on the maximum number of PHREEQC simulations allowed in an input file (was 1000).
- Added a new keyword, 'overlay'. This enables the main plot file to be over-plotted with a second plot file. Useful for predominance diagrams, watermarking etc. See `demo\Fe\hfo_with_overlay\hfo.aq.bat` for an example.
- Added the possibility of late changes to label positions using `labels.set` and `dlabels.set` files. See Section 7.5.2 in the Guide and the above example.
- Removed a bug when input files containing more than 1000 lines or so, or with very long lines, failed to substitute some tags.
- If `fitMethod` contains a list of different methods, then a plot will now be produced for each one.
- Added 'An Introduction to PhreePlot's looping' to \doc folder.
- Updated to [Phreeqc_3.3.5_10806](#).