Re: PHREEQC3 manual (comments)

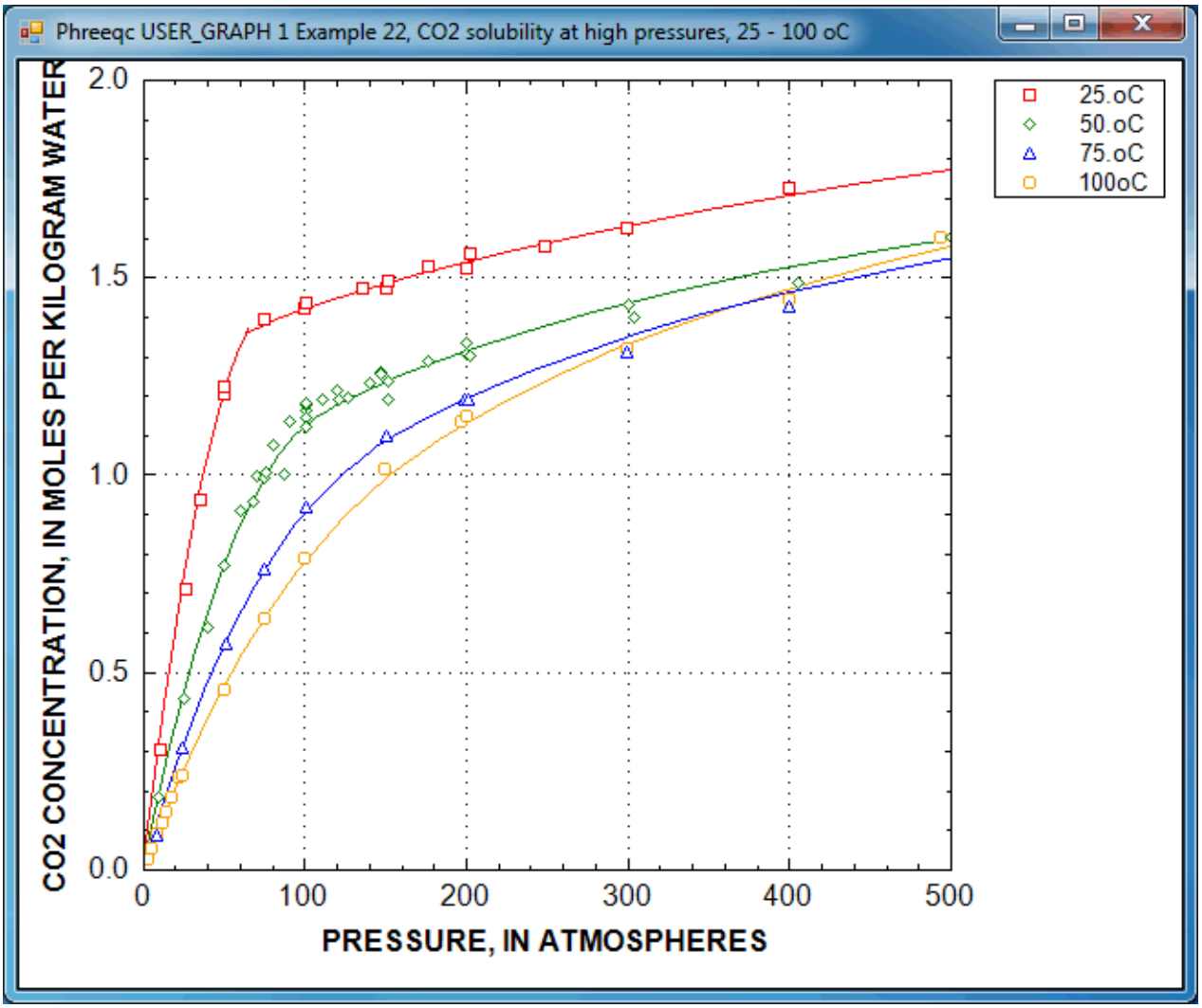
David L Parkhurst to: david 06/14/2012 11:15 AM

Hi David,

Your comments on the manuscript are greatly appreciated. Thanks for taking the time for a careful read.

The long delay is largely due to a significant rewrite of the code. It was getting pretty cluttered with obsolete #ifdefs for C compilation, which made parts of the code unreadable. I also converted the "reactants" (solutions, equilibrium_phases, surface, and others; anything identified with a user number) from C to C++, which should make it easier to implement the code in other software.

We (really Tony) have also added high-pressure capabilities. Molar volumes are now defined in the databases phreeqc.dat and pitzer.dat, which allow equilibrium constants to be calculated as a function of pressure. A Peng-Robinson fugacity coefficient is available for gases, which allows for non-ideal gas calculations. (Lots of new possibilities for PHREEPLOT).



It has also taken quite a while just to work through comments, work on consistency, check the examples, insert the figures, complete the Contents, and so on. It will never be right, but I think it is good enough. So

thanks for all the errors that you caught.

You also asked for some changes in USER_GRAPH, which I implemented. You were right that the red boxes were irrelevant and the background may not look good when charts were written to file, and a batch option is needed. Now, when a graph is written to file, red boxes for chart options are omitted. I added a batch option, which automatically closes the chart at the end of the run. If an additional file name is given, then the chart is written to file in the format given by the file extension (emf, jpg, gif, etc). If an additional boolean value is given, the background color is retained or omitted. It is also possible to toggle the background and red boxes interactively with the chart options (right-click options). Thanks for pointing out the deficiencies.

I think we can make versions of IPhreeqc with all of the new capabilities, except charting. I'm not sure what we will do with charting because it requires .NET to be installed. We have included charting in PhreeqcI (GUI), but will require .NET to be installed first. I will try to send you the latest sometime next week. We added a few more methods to the IPhreeqc module to handle output more consistently. Old methods are unchanged.

Summer is very pleasant here and the living is easy. Renee has her garden in (after replacing some plants damaged by hail). Hope you are well in England and can avoid most of the crush of the Olympics.

Thanks again for your time,

David


phreeqc3_editorial.pdf


KinniburghCommentReply.pdf

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david | David & Tony Well done on a great job. PHREE... | 10/03/2011 03:33:10 AM

From: david@phreeplot.org
To: dlpark@usgs.gov
Date: 10/03/2011 03:33 AM
Subject: PHREEQC3 manual (comments)

David & Tony

Well done on a great job. PHREEQC goes from strength to strength. I have only run a couple of
examples with the new version so have a lot of exploring to do. Look forward to doing that over the
winter.

I did read the Appendix but haven't tried any of the _MODIFY keywords yet. Would these speed up
grid-type calculations (like I use for contouring) by enabling better initial estimates to be made?

I have listed comments whenever the text caused me to pause for more than a microsecond - most of
these are trivial typos and possibly Anglo-American style diffs.

Good luck with getting this task completed...

David

[attachment "phreeqc3_draft_comments(dgk).pdf" deleted by David L Parkhurst/WRD/USGS/DOI]