Comments on phreeqc3_draft.pdf, Last modified 12:22 2/8/11

Whole document read/scanned. Links not all checked but the few tested worked ok. References and reference list not checked for consistency.

pdf page(s)	PHREEQC page(s)	Comment
4		line 5: 2011 not 2010
16-19	xiv - xvii	Check all figure captions for loss of superscripts, e.g. 22Na, Na+, Cl-, 36Cl- etc
16-19	xiv - xvii	Double? line spacing of list of Figures seems too wide and contrasts with single? spacing of List of Tables. Spacing of table of Contents seems about right.
27 line3		but ion fluxes -> but where ion fluxes
27		You refer to PHREEQE but not PHREEQC version 2. I wonder whether you should say in the second sentence of the Abstract something like 'It updates PHREEQC version 2 (P&A,1999)'. Or is that self-evident?
446	422	Footnote says 'PHAST Version 2'
29	5	Strong and weak sites are not a necessary part of the DLM or CD_MUSIC
29	5	para 3: which activity - surface or solution? Not that clear.
30	6	line-7: defining - > define
31	7	line 11: to the program -> by the program
32	8	'The ion exchange model assumes that the thermodynamic activity' - it is the IE formulation and data in the databases that assume this, not the model per se.
33	9	Transport Modelling, line 4: ? in the many cases -> in many cases
35	11	last para, line 2: -> until it reaches an END keyword or the end of the file.
36	12	para 1: -> provides total concentrations of elements in solution.
	12	last para: -> one or more types of complexation sites
38	14	para 2 line 10: bold 'Examples'
43	19 etc	para 1, line 3: ? table 1 etc (lc 't' - bit unusual though it is consistent throughout, like 'equation'. USGS format?)
52	27	last line: -> table 3 (delete 'table')
53	29	Phosphorous -> Phosphorus
55	31	line -3: next <higher> numbered cell (depends on direction of flow)</higher>
59	35	para 3: Solution <0> is the infilling solution (depends on direction of flow). Also see bottom of page.
126	102	line -10: -> the <absolute> difference between two estimates</absolute>
136	112	Notes line 1: ?previous versions <of> PHREEQE and PHREEQC</of>

146	122	Example data block 1: Line 5 Line 1b line break missing
148	124	line -8: -> in an equation <to> designate liquid water</to>
162	138	Line -13: sold_solutions -> species
180	156	Notes para 2 line 8: should steps " be in bold since the word 'steps' is not actually required in REACTION?
180	156	line -9, 'has as set of cells numbered': as -> a
		line -6, 'in the IPhreeqc are': missing 'module'?
244	220	line -7: Identifier <for> CD-MUSIC (missing 'for')</for>
254	230	line -4: per cubic meter) : missing)
259	235	lines 6 & 8: thermodynamical potential -> thermodynamic potential
262	238	line 1: missing space after 'coefficients.'
270	246	line -6 etc : tic marks -> tick marks (I'm scratching my head on this one!)
272	248	line -13: , 2011) If (missing full stop?)
284	260	line 1 after graph: missing 'and'?
		line 2: -> 0< >to 360 (missing space)
289	265	check that MISC1 and MISC2 both refer to component 2
304	280	line -1: CELCIUS -> CELSIUS. Also Title doesn't match input.
305	281	Figure 4 et al: my fig is coloured v light yellow in lower rh triangle? Seems to be a feature of the rendering of a light yellow background gradient by FM. Is this gradient user-definable - i.e. can I turn it off?
		When you Save/Print an image, should not the prompts - 'Click right mouse' and 'Press Alt + F4' be omitted from the saved image?
		Is it possible to specify closing the plot window(s)/saving images etc from within the input file to make plot production more batch-friendly?
328	304	line -8: in English English we say: In <the> case of a</the>
331	307	USER_GRAPH: is '1' (the graph number) missing or is it optional?
333	309	line -5: surface charge (why colon?)
334	310	line 3: I don't think 'strong and weak sites' per se are a necessary or defining aspect of the CD-MUSIC model. There can be any number of 'sites' (1, 2, 3 or more) with distinct binding characteristics.
334	310	para 2: I think it would be more accurate to say ' <initially> developed for sorption on goethite'. The initial intention was always to develop a general model for oxides though it was initially tested with goethite. Now many other oxides have been tested.</initially>
336	312	Not sure why the first two simulations (see below) haven't been commented out - they are not necessary? USE solution 1 USE surface 1 EQUILIBRIUM_PHASES 1 Fix_H+ -5.0 NaOH 10.0 END

		USE solution 1 USE surface 1 EQUILIBRIUM_PHASES 1 Fix_H+ -5.25 NaOH 10.0 END # and so on
355	331	line -8: 'in an astonishingly good agreement'. Delete 'an'.
357	333	axis_titles: CELCIUS -> CELSIUS (also plot)
360	336	line -3: ? decrease in -> decrease
373	349	line 2: ppm., -> ppm,
381	357	line -7: Nta.(mol/L) - delete full-stops
382	358	line before Table 42: missing full-stop at end of sentence
394	370	para 2: limits (while minimizing - delete (
494	446	Christensen, TH (1984): 'at low concentration(s)' - duplicated
		Daveler reference: improve line break