

**Particle swarm optimization for the estimation of surface complexation constants
with the geochemical model PHREEQC-3.1.2**

MS No.: gmd-2017-38

No	Page	Line	Suggested Correction	Remarks
1	1	10	..process in water treatment,	
2	1	16	..was used for the first time...	
3	1	17	..thermodynamic parameters identified...	
4	1	19	..when both softwares are coupled to PHREEQC...	
5	2	30	..has been applied in a.....	
6	2	36	..estimate the coefficients of permeability..	
7	2	41	..model such as PHREEQC..	
8	2	44	..basic PSO principles....	
9	2	45	..in 1995 (source).	Include the source of information
10	2	45-46	..However, in this study the current Standard Particle Swarm Optimization proposed by Clerk (2012) and Zambrano-Bigiarini et al (2013) was used. The code known as SPSO2011 was used in the ..	Recast as indicated
11	2	49-50	In addition, the functions for plotting in....	
12	2	51	..The source...../hydroPSO	Place after line 59 page 3
13	3	57	..estimation in geochemical models..	
14	3	59	..PEST by Doherty (2010) and Nair et al (2014)	
15	3	60-76		Why the highlights?
16	3	61	..PEST uses the Gauss-...	
17	3	63	..algorithm that initially..	
18	3	64	..matrix is then used..	
19	3	65	..to obtain a small function value..	Check
20	4	81	..(M equals Ca, Mg, Sr) obtained	
21	4	90	..different types of SCMs such as..	

22	4	92	..(modified TLM). In this work, ...	
23	4	102		This is hanging. Any link with line 103?
24	5	106	..pH value of between 6.5 and 9.0	
25	5	110	..on quartz decreased to 50, 30 and 10% respectively (Nair and Merkel, 2011)	
26	5	112	..6 parameters used to calibrate..	
27	5	113	..Nair et al. (2014)	
28	6	117	..Issue for users..	
29	6	118-120	..Particle Swarm Optimization.....disciplines.	Check with lines 26-27 page 1
30	6	122	..and collective previous studies.	
31	6	125	..following specific equations to the selected PSO version, finding the minimum or (maximum) value of user-defined objective function (..)	Check this again
32	6	128	..hydroPSO was used to improve them with a single software.	
33	6	129	..hydroPSO uses six PSO variants, four topologies, two initialization of particles position and five alternatives for initializing particles velocities among other fine-tuning options (.....)	
34	6	138	..which uses..	
35	7	142	..(Poeter et al., 2005; Abudelaziz and Merkel, 2015), relative to PEST software	
36	7	144	..optimization engine. These files include: (i) ..	
37	7	150-151	..was slightly modified..	
38	7	151-157		Is the highlights footnotes?
39	7	157	..are required. These include: i)	
40	7	162-163		Add source of the Manuel
41	7	163-165	..Figures 1a, b	Harmonize with lines 151-157
42	8	167-169 172-176		Why the highlights?

43	8	179-181	..More information.....and Rojas (2013)	Repeated Check
44	8	185-186	..One.....(.....model).	Remove
45	8	188	r^2	
46	8	189	(Figure 2)	Remove
47	10	196-203	In hydroPSO.....achieved.	This should be part of Computational Implementation
48	11	211	..Figure 4 presents values of	
49	11	213	..samples during the optimization, respectively	Repeated see line 211 page 11
50	12	221-223 224-229		Harmonize these two sections, they present the same information
51	12	228	Figure 5 was used to identify.....model performances.	
52	13	235	Figures 6 and 7	
53	13	238	while,	
54	13-14	238-239	At the top of figure 6	
55	18	249	Figure 8 Correlation....	
56	20	256-260		Why bold? Footnotes or part of caption for Figure 8?
57	20	261		Hanging
58	20	265-266		Where are equations 1-6. Are there part of Table 1. Then label them properly
59	21	275	..data, it can be shown that the log k values.....	