Hand in 2, Eirik Storrud Røsvik

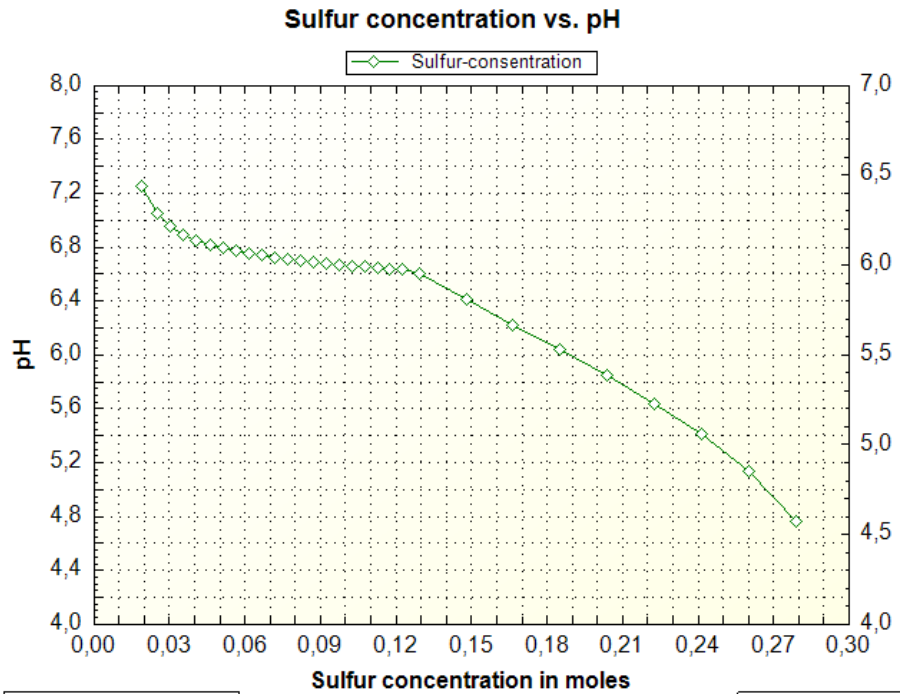
Task 1

A and B answered in input file/exercise2.xls (Table 1)

C)

By observing the printout in Table 1, the d_pyrite and d_calcite values corresponds to the amount of dissolved pyrite and calcite respectively. From the table, at step 1, -0.0095 moles of pyrite and 0.014289 moles of calcite has been dissolved.

D)



E/F)

Observing Table 1, the last step to contain undissolved calcite is step 21 (column named only 'calcite'). This can also be observed in the SI column (SI < 0 constitutes an undersaturated, SI=0 means saturated.) The SI number at step 21 is 0 and for step 22 SI < 0.

Observing the same numbers for pyrite, it can be observed that for step 30, there is still undissolved pyrite (column named only 'pyrite'). In the column for SI pyrite, it can again be observed that the SI = 0 for all time steps, meaning that for the entire reaction the solution of saturated with pyrite.

G)

The expected precipitate would be some form of Calcium sulfate. The first reaction produces dissolved Sulfuric acid and dissolved iron (II) sulfate:

$$FeS_{2(s)} + \frac{7}{2O_2} + H_2O \rightarrow FeSO_4 + H_2SO_4$$

The sulfuric acid will in this solution 'instantly' react with the calcite to produce carbon dioxide gas and insoluble calcium sulfate:

$$CaCO_{3(s)} + H_2SO_4 \rightarrow CaSO_{4(s)} + CO_2 + H_2O$$

As the calcium sulfate is precipitated out in a hydrous environment, the resulting precipitate is likely in hydrous form as gypsum ($CaSO_4$*$2H_2O$) (Verron et al, 2019)

Sources:

Experimental Study of Pyrite Oxidation at 100◦C: Implications for Deep Geological RadwasteRepository in Claystone (03.06.2019) Verron, H. Sterpenich, J. Bonnet, J. Bourdelle, F. Mosser-Ruck, R. Lorgeoux, C. Randi, A. Michau, N.

Appendix:

Table 1 (Selected values from Exercise2.xls)

step	pH	pyrite	d_pyrite	calcite	d_calcite	si_pyrite	si_calcite
0	7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-999.999	-999.999
1	6.43635	2.90E-01	-9.52E-03	2.86E-01	-1.43E-02	0	0
2	6.28003	2.81E-01	-1.90E-02	2.72E-01	-2.75E-02	0	0
3	6.21002	2.71E-01	-2.86E-02	2.59E-01	-4.08E-02	0	0
4	6.1658	2.62E-01	-3.81E-02	2.46E-01	-5.42E-02	0	0
5	6.13434	2.52E-01	-4.76E-02	2.32E-01	-6.77E-02	0	0
6	6.11027	2.43E-01	-5.71E-02	2.19E-01	-8.12E-02	0	0
7	6.09094	2.33E-01	-6.67E-02	2.05E-01	-9.48E-02	0	0
8	6.07487	2.24E-01	-7.62E-02	1.92E-01	-1.08E-01	0	0
9	6.06114	2.14E-01	-8.57E-02	1.78E-01	-1.22E-01	0	0
10	6.04919	2.05E-01	-9.52E-02	1.64E-01	-1.36E-01	0	0
11	6.0386	1.95E-01	-1.05E-01	1.51E-01	-1.49E-01	0	0
12	6.0291	1.86E-01	-1.14E-01	1.37E-01	-1.63E-01	0	0
13	6.02047	1.76E-01	-1.24E-01	1.23E-01	-1.77E-01	0	0
14	6.01258	1.67E-01	-1.33E-01	1.09E-01	-1.91E-01	0	0

15	6.00529	1.57E-01	-1.43E-01	9.54E-02	-2.05E-01	0	0
16	5.99852	1.48E-01	-1.52E-01	8.15E-02	-2.18E-01	0	0
17	5.9922	1.38E-01	-1.62E-01	6.77E-02	-2.32E-01	0	0
18	5.98625	1.29E-01	-1.71E-01	5.38E-02	-2.46E-01	0	0
19	5.98065	1.19E-01	-1.81E-01	3.99E-02	-2.60E-01	0	0
20	5.97533	1.10E-01	-1.90E-01	2.59E-02	-2.74E-01	0	0
21	5.97029	1.00E-01	-2.00E-01	1.20E-02	-2.88E-01	0	0
22	5.946	9.05E-02	-2.10E-01	0.00E+00	-3.00E-01	0	-0.036
23	5.80463	8.10E-02	-2.19E-01	0.00E+00	-3.00E-01	0	-0.2898
24	5.66522	7.14E-02	-2.29E-01	0.00E+00	-3.00E-01	0	-0.5411
25	5.52464	6.19E-02	-2.38E-01	0.00E+00	-3.00E-01	0	-0.7961
26	5.37931	5.24E-02	-2.48E-01	0.00E+00	-3.00E-01	0	-1.0618
27	5.22432	4.29E-02	-2.57E-01	0.00E+00	-3.00E-01	0	-1.3477
28	5.05177	3.33E-02	-2.67E-01	0.00E+00	-3.00E-01	0	-1.6698
29	4.84644	2.38E-02	-2.76E-01	0.00E+00	-3.00E-01	0	-2.0585
30	4.57032	1.43E-02	-2.86E-01	0.00E+00	-3.00E-01	0	-2.5896