

Assignment of wastewater infiltration and repairing

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a) Do a speciation of the waste water without DOC. Use the Amm.dat database in PHREEQC for this entire exercise. What are the dominant species?

Table 1. Dominant species in waste water

Species	Molality	Species	Molality
AmmH+	1.22E-03	Fe(OH)2+	4.19E-07
HCO3-	2.96E-03	Fe(OH)3	3.27E-07
CO2	9.25E-04	K+	3.68E-04
Ca+2	7.82E-04	Mg+2	1.24E-04
Cl-	1.73E-03	Na+	2.24E-03
Fe+2	6.02E-06	SO4-2	2.82E-04

The dominant species in waste water are shown in Table 1. Ammonia concentration is high, and the main iron ions are listed in the table, because it is essential in the following analysis.

Now add DOC to the waste water.

b) Waste water infiltration has continued for 40 years and at around 30 m depth a Fe(II) peak of 10-15 mg/L is present. Model this situation. How much iron oxide you need? Using Table 3.4 from the lecture notes Module 6 can you delineate redox zones as a function of transport distance?

I use PHREEQC to set up this waste water infiltration model and set the amounts of equilibrating Fe(OH)3(a) as 0.00005 mol in every cell. The number of cells is set up as 81, the length of the cell is 0.375m, the number of shifts is 80, and the time step is a half year. The results of waste water infiltration in 40 years are shown in the following tables and figures.

Figure 1 shows Fe(2), S(-2), and H2S concentration change along with the transport distance after infiltrating 40 years. Table 2 lists the values of criteria components for the determination of the redox index at the last time step (40 years). Table 3 lists other component concentration distribution along with the depth.

Comparing Table 2 with the criteria table for the determination of the redox index, the reductive environment can be determined in the total 30m depth. At the upper 70 cells (up to 26m), the environment is methanogenic, since no oxygen and nitrate exist, manganese ion concentration is larger than 0.1 mg/L, little sulfate exists, and hydrogen sulfide and methane significantly exist in this part. At the last cells under 26m, the reducibility is less significant than the upper

layers, which is indicated by the pe values. This is due to less water infiltrating into the bottom layers and less time to react, which results in an uncompleted reaction. The hydrogen sulfide and methane are not produced a lot. Thus the reducibility is not very significant.

Table 2. Concentration values for determination of the redox index

Soln NO.	Dist_x m	Time s	pe	Fe (2) mg/L	O (0) mg/L	N (5) mg/L	Mn (2) mg/L	SO4-2 mg/L	m_H2S mg/L	m_CH4 mg/L
0	0	1.26E+09	-3.32161	4.65E-01	0.00E+00	0.00E+00	3.21E-01	6.55E+00	4.12E+00	4.98E-02
1	0.1875	1.26E+09	-3.51543	6.33E-12	0.00E+00	0.00E+00	3.21E-01	1.21E+00	5.46E+00	4.89E-01
10	3.5625	1.26E+09	-3.57075	7.91E-12	0.00E+00	0.00E+00	3.21E-01	5.01E-01	5.66E+00	1.28E+00
20	7.3125	1.26E+09	-3.57075	7.91E-12	0.00E+00	0.00E+00	3.21E-01	5.01E-01	5.66E+00	1.28E+00
30	11.0625	1.26E+09	-3.57075	7.91E-12	0.00E+00	0.00E+00	3.21E-01	5.01E-01	5.66E+00	1.28E+00
40	14.8125	1.26E+09	-3.57075	7.91E-12	0.00E+00	0.00E+00	3.21E-01	5.01E-01	5.66E+00	1.28E+00
50	18.5625	1.26E+09	-3.57075	7.91E-12	0.00E+00	0.00E+00	3.21E-01	5.01E-01	5.66E+00	1.28E+00
60	22.3125	1.26E+09	-3.57075	7.91E-12	0.00E+00	0.00E+00	3.21E-01	5.01E-01	5.66E+00	1.28E+00
70	26.0625	1.26E+09	-3.56846	7.90E-12	0.00E+00	0.00E+00	3.21E-01	5.01E-01	5.67E+00	1.27E+00
74	27.5625	1.26E+09	-3.14761	7.37E-12	0.00E+00	0.00E+00	3.20E-01	4.42E-01	7.35E+00	8.61E-01
75	27.9375	1.26E+09	-2.73831	1.05E-11	0.00E+00	0.00E+00	3.18E-01	3.32E-01	8.33E+00	6.03E-01
76	28.3125	1.26E+09	-2.28882	3.11E-11	0.00E+00	0.00E+00	3.13E-01	1.98E-01	8.47E+00	4.38E-01
77	28.6875	1.26E+09	-1.87806	1.56E-10	0.00E+00	0.00E+00	3.01E-01	9.19E-02	7.29E+00	3.72E-01
78	29.0625	1.26E+09	-1.54174	1.71E-09	0.00E+00	0.00E+00	2.78E-01	2.57E-02	4.01E+00	3.89E-01
79	29.4375	1.26E+09	-1.27834	2.36E+00	0.00E+00	0.00E+00	2.40E-01	7.97E-07	1.66E-04	3.44E-01
80	29.8125	1.26E+09	-0.84503	1.28E+01	0.00E+00	0.00E+00	1.89E-01	2.90E-05	5.14E-05	2.48E-03

The strange part occurs on the iron concentration compared with the criteria table. Because the environment is reductive, the ion concentration should be larger than 0.1 and increase with the reducibility enhancing as the criteria table given. However, the result of iron from PHREEQC model is opposite, which is very little in the upper reductive layer and significant in the bottom. This phenomenon can be explained by the relationship between Fe(2) and S(-2) in Figure 1 and the concentration of pyrite in Table 3. The reason is that in addition to the iron ions, the solution also contains a large number of S(-2), iron ions and sulfur ions will be deposited in the form of pyrite. The concentration of pyrite is listed in Table 3. The negative divalent sulfur ion is obtained by reduction and is first reduced to hydrogen sulfide, which is dissolved in water to form the negative divalent sulfur ion and then combines with the iron ion to form the pyrite precipitation. Therefore, the reason why there are more iron ions in the lower layer is that the reduction reaction of sulfur in the lower layer is not complete, and there are fewer negative sulfur ions in the lower layer, so the iron ions in the lower layer are retained in the solution.

These processes can be verified by the curves in Figure 1.

Ammonia is an important reducing agent in this model. The concentration of N(-3) is shown in Table 3 and keeps at a high level through all the layers. While the initial water in the aquitard does not include ammonia or other significant reductive material. Thus the influence of urban wastewater infiltration is obvious that the environment of underground water changes into a significantly reductive one.

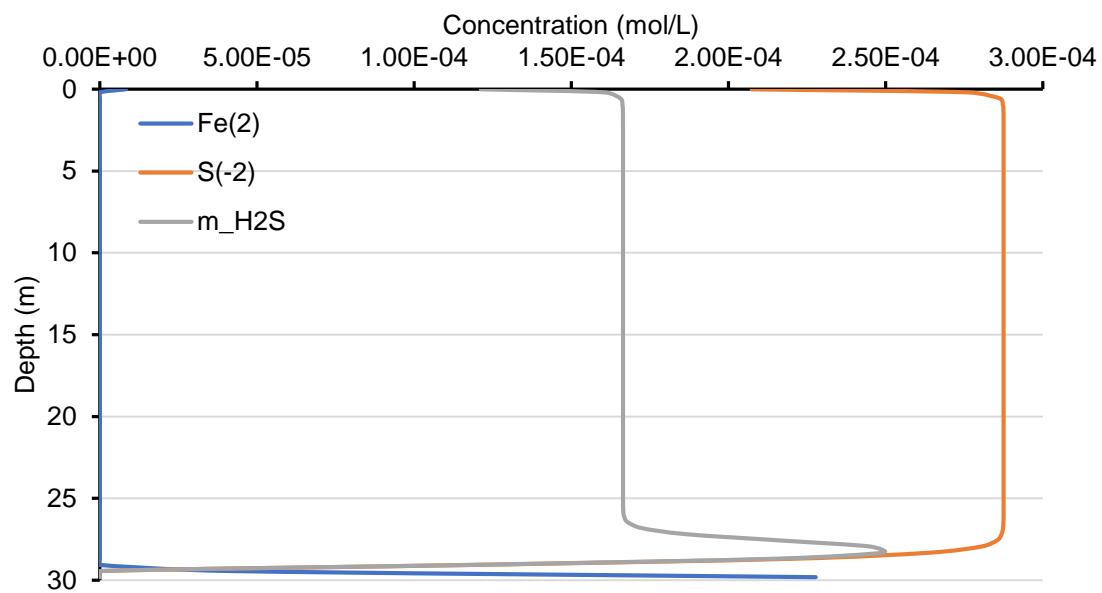


Figure 1. Three major components concentration change along with the transport distance after infiltrating 40 years

Table 3. Other components concentration distribution along the depth

Soln	Dist_x	Time	Step	pe	Fe(2)	N(-3)	S(-2)	Pyrite
No.	m	s			mol/L	mol/L	mol/L	mol/L
0	0	1.26E+09	80	-3.32161	8.31E-06	1.01E-03	2.07E-04	0.00E+00
1	0.1875	1.26E+09	80	-3.51543	1.13E-16	1.34E-03	2.76E-04	7.06E-04
10	3.5625	1.26E+09	80	-3.57075	1.41E-16	1.45E-03	2.88E-04	8.82E-06
20	7.3125	1.26E+09	80	-3.57075	1.41E-16	1.45E-03	2.88E-04	6.88E-06
30	11.0625	1.26E+09	80	-3.57075	1.41E-16	1.45E-03	2.88E-04	3.84E-06
40	14.8125	1.26E+09	80	-3.57075	1.41E-16	1.45E-03	2.88E-04	4.30E-06
50	18.5625	1.26E+09	80	-3.57075	1.41E-16	1.45E-03	2.88E-04	4.85E-06
60	22.3125	1.26E+09	80	-3.57075	1.41E-16	1.45E-03	2.88E-04	5.39E-06
70	26.0625	1.26E+09	80	-3.56846	1.41E-16	1.45E-03	2.88E-04	3.15E-06
79	29.4375	1.26E+09	80	-1.27834	4.22E-05	1.19E-03	4.93E-09	2.07E-06
80	29.8125	1.26E+09	80	-0.84503	2.28E-04	9.15E-04	1.52E-09	1.78E-10

c) The municipality has decided to stop infiltration of waste water into the

aquitard. Instead, in the area a small lake will be constructed. Assuming similar hydraulic conditions as above, how does groundwater quality develop as a function of time -say the first 80 year? Assume the lake water has the following composition.

Instead of wastewater by lake water, underground water pollution can be repaired. The groundwater quality development along time in the bottom (80 cells) is shown in Figure 2, and the details are list in Table 4. In general, there is a time lag in groundwater remediation, with the purification of relatively clean water only beginning when it seeps down into a particular aquifer. Moreover, the purification takes a certain amount of time. According to the output results of the model, the deeper the aquitard is, the longer the purification process will take. The final state of the water quality of the aquitard is close to the infiltration of the lake water. With the passage of time, the influence of sewage infiltration will become less and less. But the time it takes to get to the final state is long enough.

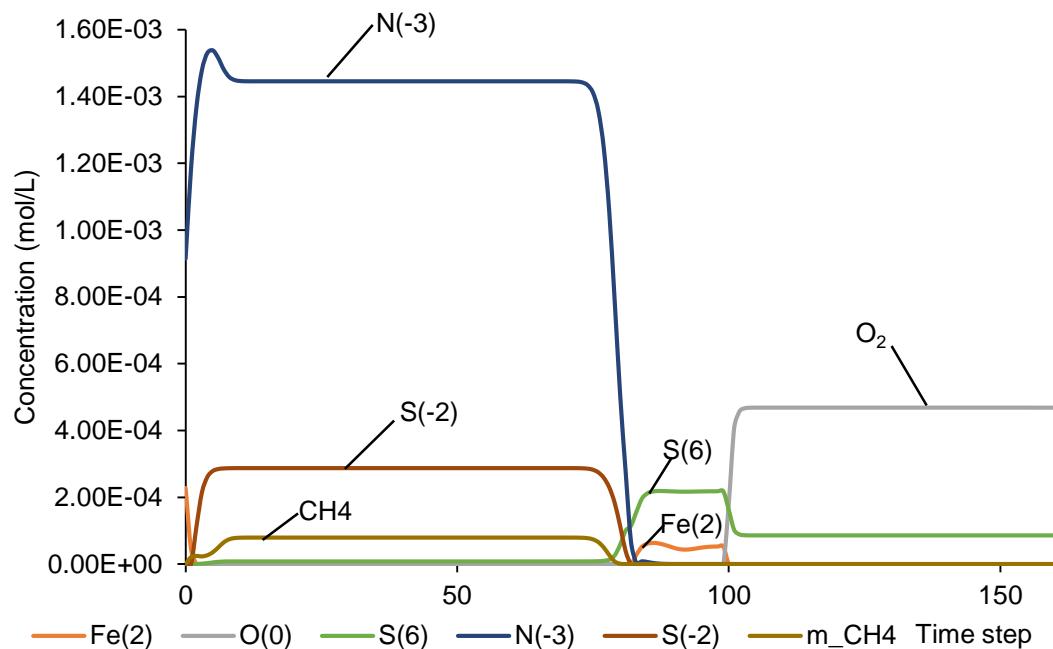


Figure 2. Water quality change in the bottom versus time

Figure 2 shows the changes in groundwater quality at a depth of 30 meters underground within 80 years of infiltration. It can be seen from the figure that in the early stage, the sewage that was infiltrated for the past 40 years is still infiltrating, the groundwater quality is further deteriorating, and the reduction of the groundwater environment continues to increase. During the fifth to seventy-fifth time periods, the water quality of this layer remained basically stable

and continued to maintain a highly reductive environment. When approaching the seventy-fifth time period, nearly forty years after the lake began to infiltrate, the impact of the lake's infiltration finally reached this aquitard, and the water quality began to improve. The reducing substances ammonium, methane, and negative divalent sulfur began to be consumed. By the time it was consumed around the 41st year, these three main reducing agents were consumed to trace amounts, so pyrite began to accelerate dissolution. Therefore, from the 41st year, the content of iron ions increased, and the content of sulfate ions increased. At this time, the groundwater environment is still a reducing environment, but the reducing ability has been significantly reduced. From the 41st year to the 50th year, oxygen and other oxidizing substances were continuously imported, pyrite was continuously dissolved, reducing substances were continuously oxidized, and the groundwater environment continued to move closer to the aerobic environment. Until the 50th year, the reducing substances in the water were exhausted, dissolved oxygen and nitrate ions appeared in the water, and the groundwater environment became an aerobic environment. Over time, due to the continuous erosion of the lake's infiltration, the water quality characteristics of this aquifer will approach the lake water quality characteristics (after kinetic reaction). The reaction process of every layer is similar to the approach above, while the differences are the beginning time of repairing and the pyrite dissolving time. In the case of the bottom layer, the repairing time is almost 51 years, which is longer than the pollution time 40 years.

Table 4. Distribution of groundwater quality in some major steps in the bottom layer

Step No.	pe	Fe(2) mol/L	O(0) mol/L	N(5) mol/L	Mn(2) mol/L	S(6) mol/L	N(-3) mol/L	S(-2) mol/L	m_CH4 mol/L	Pyrite mol/L
0	-0.84503	2.28E-04	0.00E+00	0.00E+00	3.43E-06	4.73E-10	9.15E-04	1.52E-09	1.55E-07	1.78E-10
1	-1.27559	4.50E-05	0.00E+00	0.00E+00	4.35E-06	1.27E-11	1.19E-03	4.78E-09	2.11E-05	2.02E-06
10	-3.56533	1.41E-16	0.00E+00	0.00E+00	5.84E-06	8.10E-06	1.45E-03	2.88E-04	7.93E-05	3.53E-06
20	-3.57075	1.41E-16	0.00E+00	0.00E+00	5.84E-06	8.11E-06	1.45E-03	2.88E-04	7.97E-05	3.53E-06
30	-3.57075	1.41E-16	0.00E+00	0.00E+00	5.84E-06	8.11E-06	1.45E-03	2.88E-04	7.97E-05	3.53E-06
40	-3.57075	1.41E-16	0.00E+00	0.00E+00	5.84E-06	8.11E-06	1.45E-03	2.88E-04	7.97E-05	3.53E-06
50	-3.57075	1.41E-16	0.00E+00	0.00E+00	5.84E-06	8.11E-06	1.45E-03	2.88E-04	7.97E-05	3.53E-06
60	-3.57075	1.41E-16	0.00E+00	0.00E+00	5.84E-06	8.11E-06	1.45E-03	2.88E-04	7.97E-05	3.53E-06
70	-3.57075	1.41E-16	0.00E+00	0.00E+00	5.84E-06	8.11E-06	1.45E-03	2.88E-04	7.97E-05	3.53E-06
80	-3.26105	1.07E-16	0.00E+00	0.00E+00	2.78E-06	5.80E-05	5.07E-04	1.14E-04	1.30E-06	3.53E-06
90	0.932451	4.82E-05	0.00E+00	0.00E+00	6.40E-07	2.17E-04	4.07E-08	2.26E-09	9.67E-19	4.94E-06
100	16.5612	3.70E-11	1.80E-04	2.51E-15	6.40E-07	1.63E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00

110	15.0259	1.49E-14	4.69E-04	5.10E-24	6.40E-07	8.60E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
120	15.0263	1.49E-14	4.69E-04	0.00E+00	6.40E-07	8.60E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
130	15.0335	1.47E-14	4.69E-04	0.00E+00	6.40E-07	8.60E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
140	15.0855	1.35E-14	4.69E-04	0.00E+00	6.40E-07	8.60E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
150	15.2491	1.02E-14	4.69E-04	0.00E+00	6.40E-07	8.60E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
160	15.5105	6.41E-15	4.69E-04	0.00E+00	6.40E-07	8.60E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00

In conclusion, this model describes the groundwater quality changes in the processes of wastewater infiltration in the first 40 years and repairing by fresh lake water in the following 80 years. The results of this model indicate the wastewater can cause the groundwater into an oxygen-free reductive environment, and the repairing time is longer than the pollution time.