

Table 1 Mineral composition of aquifer sediment at different depths in the shallow aquifer (weight percentage).

Depth (m)	Quartz	Microcline	Illite	Kaolinite	Albite
61.26	38.76	17.5	19.74	20.85	3.15
67.97	81.86	9.26	1.64	5	2.24
69.49	59.35	17.27	2.79	18.16	2.43
70.10	32.84	18.46	14.39	32.96	1.35
71.02	50.93	20.91	5.31	21.76	1.09

Table 2. Mass balance calculation of major ions for push-pull test (unit: g).

Ions	M_{inj}	M_{bkg}	M_{mix}	M_r	M_T	$\left \frac{M_r}{M_T} \right \times 100\%$
Br	436.1	0	436.1	0	436.1	-
Ca	74.7	217.3	292.0	5.2	297.2	1.7
Mg	31.3	92.6	123.9	2.5	126.4	2.0
Na	161.4	131.3	292.7	3.2	295.9	1.1
K	5.2	15.3	20.5	0.5	21.0	2.4
Si	51.3	158.5	209.8	15.9	225.7	7.0
Cl	98.7	295.6	394.3	-11	383.3	3.3
SO4	3.8	10.6	14.4	-0.2	14.2	1.4
NO3	14.8	44.7	59.5	-0.6	58.9	1.0

Note: M_{inj} , M_{bkg} , M_{mix} , M_r , and M_T explained in text of Section 3.

Table 3. Mass balance calculation of trace metals for push-pull test (unit: mg).

Ions	M_{inj}	M_{bkg}	M_{mix}	M_r	M_T	$\left \frac{M_r}{M_T} \right \times 100\%$
Al	4.6	7.2	11.8	1453.7	1465.5	99.2
As	0.8	1.7	2.5	1.0	3.5	28.6
B	48.4	111.3	159.7	2.2	161.9	1.4
Ba	264.5	770.2	1034.7	96.3	1131	8.5
Bi	0.1	0.01	0.11	0.5	0.61	82.0
Cd	0.7	2.3	3	1.3	4.3	30.2
Co	2.81	8.98	11.79	8.23	20.02	41.1
Cr	0.3	1.3	1.6	1.7	3.3	51.5
Cu	3.0	1.7	4.7	0.8	5.5	14.5
Fe	6.8	19.4	26.2	613.9	640.1	95.9
Mn	5.4	14.6	20	18.2	38.2	47.6
Mo	3.2	1.5	4.7	-0.4	4.3	9.3
Ni	10.9	34.0	44.9	16.4	61.3	26.8
Pb	0.1	0.05	0.15	1.5	1.7	90.9
Rb	12.1	36.5	48.6	3.6	52.2	6.9
Se	4.2	4.6	8.8	0.6	9.4	6.4
Sr	284.3	835.5	1119.8	27.1	1146.9	2.4
Ti	9.7	30.1	39.8	47.9	87.7	54.6
U	0.2	0.4	0.6	0.8	1.4	57.1
V	0.9	2.7	3.6	2.0	5.6	35.7
Zn	43.6	161.7	205.3	-17.4	187.9	9.3

Note: M_{inj} , M_{bkg} , M_{mix} , M_r , and M_T explained in text of Section 3.

Table 4 Comparison of overall reaction rates of ion in batch experiment and push-pull test.

Major ions (mg/L/h)									
Ions	Ca	Mg	Na	K	Si				
Batch experiment	0.106	0.049	0.016	0.014	0.061				
Push-pull test	0.021	0.01	0.013	0.002	0.064				
Trace metals (µg/L/h)									
Ions	Al	As	B	Ba	Cd	Co	Cr	Cu	Mn
Batch experiment	0.656	-0.01	0.071	1.239	0.011	0.74	-	0.01	1.33
Push-pull test	5.85	0.004	0.008	0.39	0.005	0.033	0.007	0.003	0.067
Ions	Fe	Mo	Ni	Pb	Se	Sr	U	V	Zn
Batch experiment	-	-0.06	0.449	-	-0.02	0.369	0.001	-0.04	-
Push-pull test	2.47	-0.02	0.066	0.006	0.002	0.108	0.003	0.008	-0.07

Table 5. Comparison of maximum concentrations observed in push-pull test with concentration measurements from 14 wells at Cranfield shallow aquifer.

Statistics of concentration measurements ²							
Ions	Unit	Max Conc. ¹	Min	25% ³	50% ⁴	75% ⁵	Max
pH	-	5.0 ⁶	5.3	6.2	6.4	6.6	7.5
Alkalinity ⁷	mg CaCO ₃ /L	80.9	30.0	60.8	86.0	104.6	154.3
DIC ⁸	mmol/L C	35.25	1.3	1.9	3.1	3.7	5.5
δ¹³C of DIC	‰	-38.1 ⁹	-21.3	-18.7	-17.9	-15.8	-11.4
Ca	mg/L	22.3	4.0	8.5	19.5	22.3	27.9
Mg	mg/L	9.4	1.6	2.4	7.9	9.0	10.2
K	mg/L	1.5	1.1	1.6	1.8	2.8	8.4
Na	mg/L	-	7.6	9.1	11.9	30.2	74.3
Si	mg/L	19.5	1.9	11.1	14.9	17.8	23.0
Ba	µg/L	104.3	10.0	31.8	125	176.3	258.0
Cu	µg/L	0.9	<3.0	3.56	5.0	9.0	34.0
Fe	mg/L	0.2	<0.007	0.04	0.6	1.7	11.2
Mn	µg/L	13.4	1.0	11.5	107	161.5	708.0
Zn	µg/L	20.2	3.0	9.8	19.0	25.0	1187.0

Note:

¹Maximum concentration of an ion observed during pulling phase of push-pull test.

²Concentration measurements include all measurements for water samples collected from 14 wells (Figure 1) from August 2008 through March 2012.

³25% = first quartile, ⁴50% = second quartile, and ⁵75% = third quartile.

⁶Minimum pH values selected because $\text{pH} = -\log([\text{H}^+])$

⁷Alkalinities= field measurements

⁸Dissolved inorganic carbon (DIC) measured using Tekmar Dohrman Phoenix 8000 system except the maximum DIC which was estimated in the mixing model.

⁹Smallest δ¹³C of DIC observed for the push-pull test