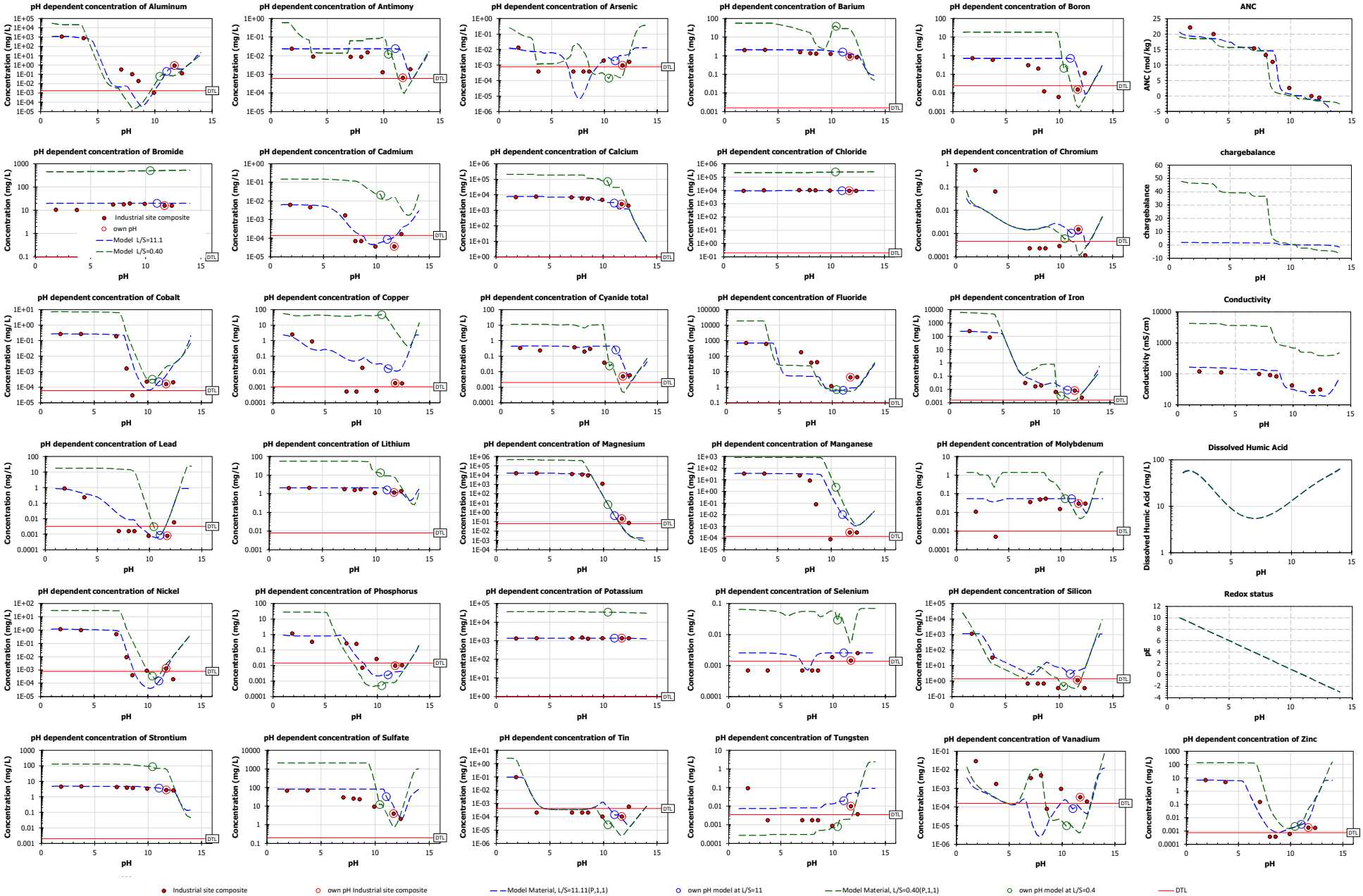
Contaminated Industrial site

COMPARISON pH DEPENDENCE DATA WITH MODEL



Object pH Dependent Leaching Test Model
Name Industrial F contaminated site

pH Dependent Leaching Test Scenario

Lab Test

Extra L/S Simulation

Lab Test

Model Parameters

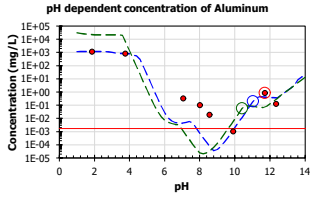
Entity	Unit	Default	Available Content Entity	mg/kg	Entity	mg/kg	Entity	mg/kg
c0		-5.030	Al	1.319E+04	Fe	2728	PO4	40.75
c1		0.7637	As	0.1499	B	8.271	Sb	0.2662
c2		-0.3660	Ba	23.40	Si	1.271E+04	Se	0.02844
c3		0.05515	Br	221.7	Hg	2.006E-07	Sn	1.069
c4		-0.003379	Ca	8.557E+04	K	1.524E+04	SO4	929.5
c5		7.446E-05	Cd	0.07052	Li	23.40	Sr	53.48
Clay	mg/kg	1.900E+04	Cl	1.046E+05	Mg	1.860E+05	Th	2.320E-07
Hydrous Ferric Oxide	mg/kg	180.0	CNT	5.001	Mn	390.3	U	2.380E-07
L/S	L/kg	11.11	Co	3.075	Mo	0.6076	V	0.3282
pE		-0.5000	CO32-	5.010E+04	Na	2.221E+04	W	1.0000
pH		11.50	Cr	5.834	Ni	13.31	Zn	75.39
Solid Humic Acid	mg/kg	2.160E+04	Cu	28.61	NO3	210.0		
Simulated Low L/S	L/kg	0.4000	F	7784	Pb	9.780		

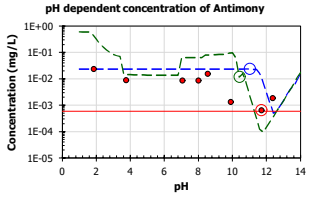
Solid Solutions

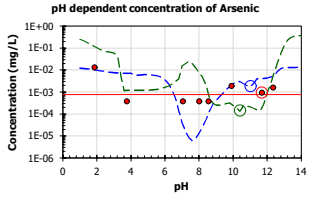
Name	End Member	Log(K)	Reaction
ettr_ss	AsO4_Ettringite_ss	26.79	AsO4_Ettringite_ss + 1 H+ + 8 H2O -> 2 Al[OH]4- + 3 AsO4-3 + 6 Ca+2 + 1 ettr_ss
	Ba_Ettringite_ss	4.008	Ba_Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ba+2 + 3 SO4-2 + 1 ettr_ss
	BO3_Ettringite_ss	-46.87	BO3_Ettringite_ss + 7 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 H2BO3- + 1 ettr_ss
	CrO4_Ettringite_ss	-8.592	CrO4_Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 CrO4-2 + 1 ettr_ss
	Ettringite_ss	-10.99	Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 SO4-2 + 1 ettr_ss
	Li-Ettringite_ss	-5.699	Li-Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 5 Ca+2 + 2 Li+ + 3 SO4-2 + 1 ettr_ss
	MoO4_Ettringite_ss	-9.592	MoO4_Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 MoO4-2 + 1 ettr_ss
	Sb[OH]6-_Ettringite	-33.80	Sb[OH]6-_Ettringite_ss + 7 H+ + 17 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 Sb[OH]6- + 1 ettr_ss
	SeO4-2_Ettringite_s	4.408	SeO4-2_Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 SeO4-2 + 1 ettr_ss
	Sn[OH]4-2_Ettringit	-69.18	Sn[OH]4-2_Ettringite_ss + 8 H+ + 4 H2O -> 2 Al[OH]4- + 6 Ca+2 + 2 SO4-2 + 1 Sn+2 + 1 ettr_ss
	Sr_Ettringite_ss	4.008	Sr_Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 3 SO4-2 + 6 Sr+2 + 1 ettr_ss
	VO3_Ettringite_ss	-53.79	VO3_Ettringite_ss + 13 H+ + 2 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 VO2+ + 1 ettr_ss
	WO4_Ettringite_ss	-9.592	WO4_Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 WO4-2 + 1 ettr_ss

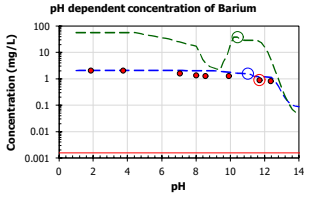
Minerals

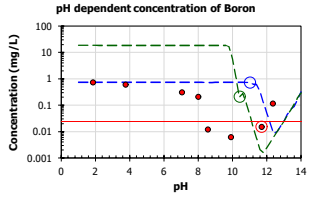
Name	Log(K)	Reaction
AA_2CaO_Al2O3_SiO2_8H2O[s]	18.18	AA_2CaO_Al2O3_SiO2_8H2O[s] -> 2 Al[OH]4- + 2 Ca+2 + 3 H2O + 1 H2SiO4-2
AA_2CaO_Fe2O3_SiO2_8H2O[s]	22.49	AA_2CaO_Fe2O3_SiO2_8H2O[s] -> 2 Ca+2 + 2 Fe[OH]4- + 3 H2O + 1 H2SiO4-2
AA_3CaO_Al2O3_CaCO3_11H2O[s]	-24.52	AA_3CaO_Al2O3_CaCO3_11H2O[s] + 4 H+ -> 2 Al[OH]4- + 1 CO3-2 + 4 Ca+2 + 9 H2O
AA_Brucite	-16.84	AA_Brucite + 2 H+ -> 2 H2O + 1 Mg+2
AA_Calcite	9.481	AA_Calcite -> 1 CO3-2 + 1 Ca+2
AA_CO3-hydrotalcite	-4.852	AA_CO3-hydrotalcite + 4 H+ -> 2 Al[OH]4- + 1 CO3-2 + 6 H2O + 4 Mg+2
AA_Magnesite	9.359	AA_Magnesite -> 1 CO3-2 + 1 Mg+2
AA_Portlandite	-22.80	AA_Portlandite + 2 H+ -> 1 Ca+2 + 2 H2O
AA_Tobermorite-I	23.86	AA_Tobermorite-I -> 2 Ca+2 + 0.8 H+ + 1.2 H2O + 2.4 H2SiO4-2
Albite[low]	85.27	Albite[low] + 8 H2O -> 1 Al[OH]4- + 6 H+ + 3 H2SiO4-2 + 1 Na+
Antimocrandallite-exp	63.00	Antimocrandallite-exp + 8 H2O -> 3 Al[OH]4- + 1 Ca+2 + 3 H+ + 2 Sb[OH]6-
Arsenocrandallite-therm	95.56	Arsenocrandallite-therm + 6 H2O -> 3 Al[OH]4- + 2 AsO4-3 + 1 Ca+2 + 7 H+
Austinite-therm	11.47	Austinite-therm + 1 H+ -> 1 AsO4-3 + 1 Ca+2 + 1 H2O + 1 Zn+2
Ba[SCr]O4[96%SO4]	9.790	Ba[SCr]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2
beta-TCP	28.93	beta-TCP -> 3 Ca+2 + 2 PO4-3
Boehmite	14.42	Boehmite + 2 H2O -> 1 Al[OH]4- + 1 H+
Ca[OH]2.Sn[OH]2	-17.00	Ca[OH]2.Sn[OH]2 + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Sn+2
Ca2Cr[OH]7.3H2O	25.30	Ca2Cr[OH]7.3H2O + 1 H2O -> 2 Ca+2 + 1 CrO4-2 + 1 H+ + 3 e-
Ca3[AsO4]2:3H2O	21.40	Ca3[AsO4]2:3H2O -> 2 AsO4-3 + 3 Ca+2 + 3 H2O
Ca3[OH]2[MoO4]2[c]	-3.000	Ca3[OH]2[MoO4]2[c] + 2 H+ -> 3 Ca+2 + 2 H2O + 2 MoO4-2
CaMoO4[c]	7.940	CaMoO4[c] -> 1 Ca+2 + 1 MoO4-2
CaSb[OH]6[s]2	18.41	CaSb[OH]6[s]2 + 6 H2O -> 1 Ca+2 + 2 Sb[OH]6-
CaWO4[c]	9.000	CaWO4[c] -> 1 Ca+2 + 1 WO4-2
Co2SiO4	6.289	Co2SiO4 + 2 H+ -> 2 Co+2 + 1 H2SiO4-2
Cuprite	6.990	Cuprite + 2 H+ -> 2 Cu+2 + 1 H2O + 2 e-
Eskolaite	139.5	Eskolaite + 5 H2O -> 2 CrO4-2 + 10 H+ + 6 e-
Fe2[MoO4]3[1]	82.02	Fe2[MoO4]3[1] + 8 H2O -> 2 Fe[OH]4- + 8 H+ + 3 MoO4-2
FeMoO4[s]	45.00	FeMoO4[s] + 4 H2O -> 1 Fe[OH]4- + 4 H+ + 1 MoO4-2 + 1 e-
Ferrihydrite	16.71	Ferrihydrite + 1 H2O -> 1 Fe[OH]4- + 1 H+
Fluorite	10.96	Fluorite -> 1 Ca+2 + 2 F-
Friedel_salt_CN-HS	-15.77	Friedel_salt_CN-HS + 4 H+ -> 2 Al[OH]4- + 2 CN- + 4 Ca+2 + 4 H2O
Manganite	-25.27	Manganite + 3 H+ + 1 e- -> 2 H2O + 1 Mn+2
Molybdocrandallite-exp	86.00	Molybdocrandallite-exp + 6 H2O -> 3 Al[OH]4- + 1 Ca+2 + 7 H+ + 3 MoO4-2
Ni[OH]2[s]	-10.80	Ni[OH]2[s] + 2 H+ -> 2 H2O + 1 Ni+2
Ni2SiO4	7.079	Ni2SiO4 + 2 H+ -> 1 H2SiO4-2 + 2 Ni+2
Pb[OH]2[C]	-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
PbMoO4[c]	15.80	PbMoO4[c] -> 1 MoO4-2 + 1 Pb+2
Sn[OH]2[s]	1.447	Sn[OH]2[s] + 2 H+ -> 2 H2O + 1 Sn+2
ZnSiO3	18.69	ZnSiO3 + 1 H2O -> 1 H2SiO4-2 + 1 Zn+2

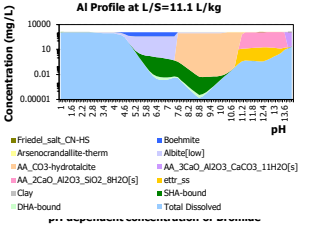

pH dependent concentration of Aluminum
Concentration (mg/L)
pH

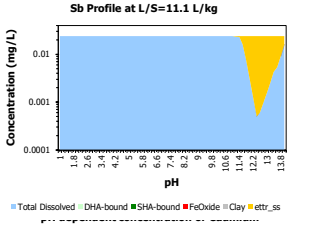

pH dependent concentration of Antimony
Concentration (mg/L)
pH

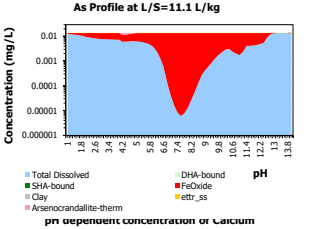

pH dependent concentration of Arsenic
Concentration (mg/L)
pH

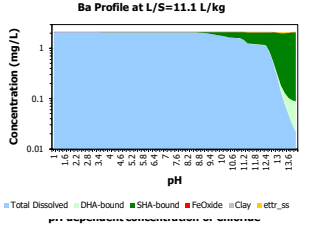

pH dependent concentration of Barium
Concentration (mg/L)
pH

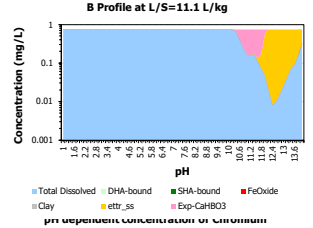

pH dependent concentration of Boron
Concentration (mg/L)
pH

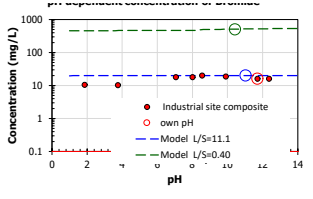

Al Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Friedel_salt_CN-HS
Boehmite
Arsenocrandallite-therm
Albite[low]
AA_CO3-hydrotalcite
AA_3CaO_Al2O3_CaCO3_11H2O[s]
AA_2CaO_Al2O3_SiO2_8H2O[s]
ettr_ss
Clay
SHA-bound
DHA-bound
Total Dissolved

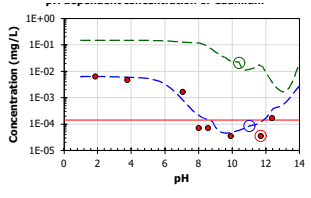

Sb Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss

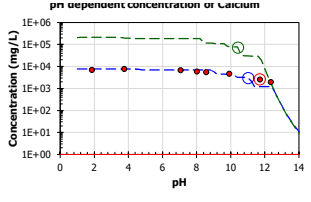

As Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss
Arsenocrandallite-therm

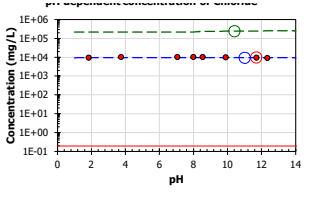

Ba Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss

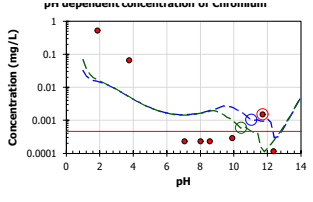

B Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss
Exp-CaHBO3

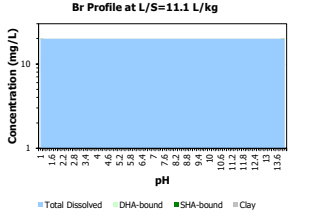

Concentration (mg/L)
Industrial site composite
own pH
Model L/S=11.1
Model L/S=0.40
pH

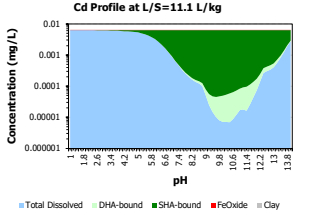

Concentration (mg/L)
pH

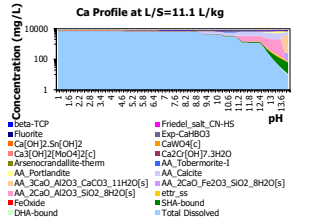

pH dependent concentration of Calcium
Concentration (mg/L)
pH

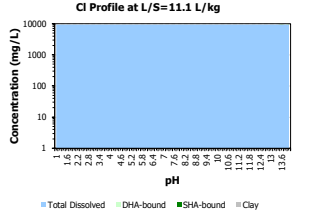

Concentration (mg/L)
pH

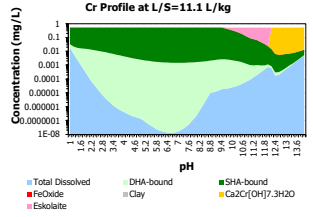

Concentration (mg/L)
pH

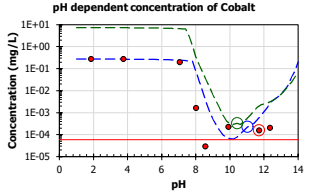

Br Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
Clay

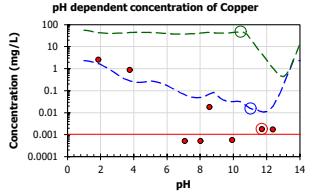

Cd Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay

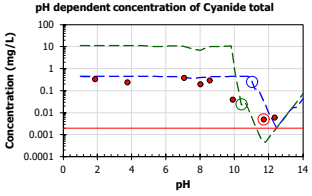

Ca Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
beta-TCP
Friedel_salt_CN-HS
Fluorite
Exp-CaHBO3
Ca[OH]2.Sn[OH]2
CaWO4[c]
Ca3[OH]2[MoO4]2[c]
Ca2C(OH)7.3H2O
Arsenocrandallite-therm
AA_Tobermorite-1
AA_Portlandite
AA_Calcite
AA_3CaO_Al2O3_CaCO3_11H2O[s]
AA_2CaO_Fe2O3_SiO2_8H2O[s]
AA_2CaO_Al2O3_SiO2_8H2O[s]
ettr_ss
FeOxide
SHA-bound
DHA-bound
Total Dissolved

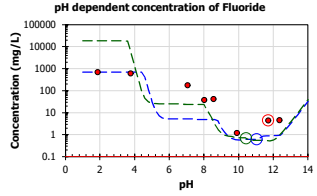

Cl Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
Clay

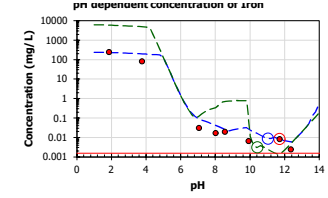

Cr Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Ca2Cr[OH]7.3H2O
Eskolaite

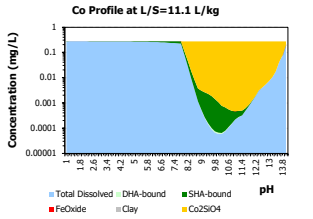

pH dependent concentration of Cobalt
Concentration (mg/L)
pH

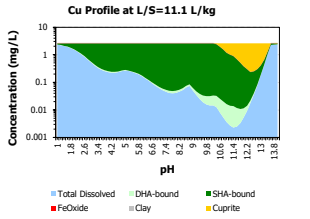

pH dependent concentration of Copper
Concentration (mg/L)
pH

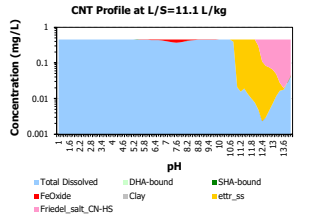

pH dependent concentration of Cyanide total
Concentration (mg/L)
pH

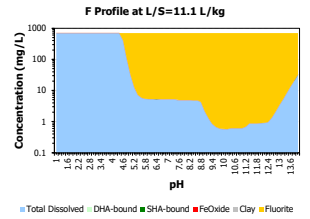

pH dependent concentration of Fluoride
Concentration (mg/L)
pH

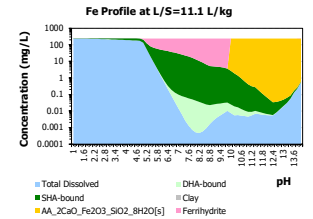

Concentration (mg/L)
pH

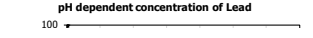

Co Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Co2SiO4

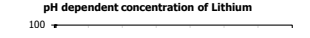

Cu Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Cuprite

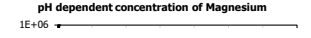

CNT Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss
Friedel_salt_CN-HS

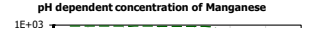

F Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Fluorite

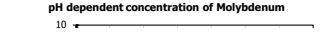

Fe Profile at L/S=11.1 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
Clay
AA_2CaO_Fe2O3_SiO2_8H2O[s]
Ferrihydrite

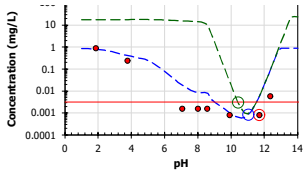

pH dependent concentration of Lead
100

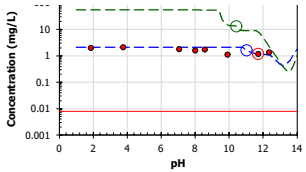

pH dependent concentration of Lithium
100

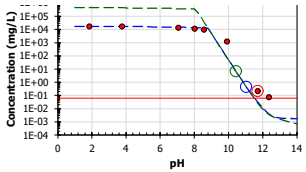

pH dependent concentration of Magnesium
1E+06

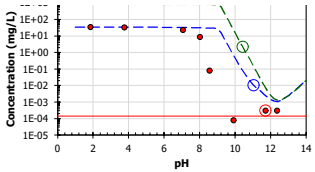

pH dependent concentration of Manganese
1E+03

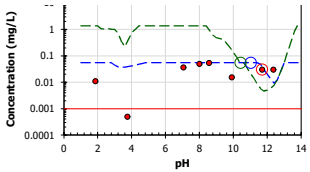

pH dependent concentration of Molybdenum
10



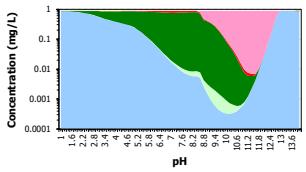




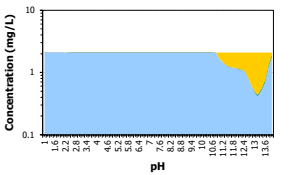




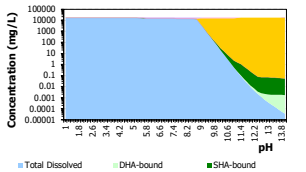
Pb Profile at L/S=11.1 L/kg



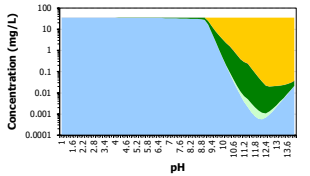
Li Profile at L/S=11.1 L/kg



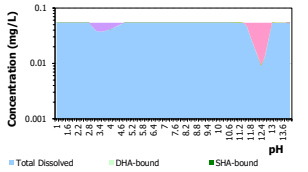
Mg Profile at L/S=11.1 L/kg



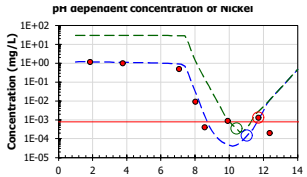
Mn Profile at L/S=11.1 L/kg



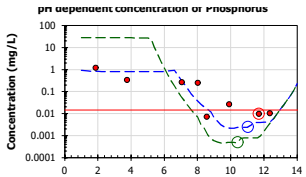
Mo Profile at L/S=11.1 L/kg



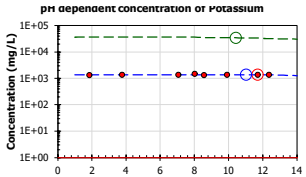
pH dependent concentration of Nickel



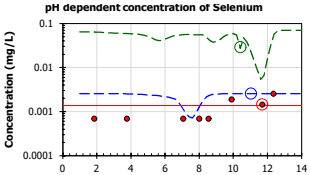
pH dependent concentration of Phosphorus



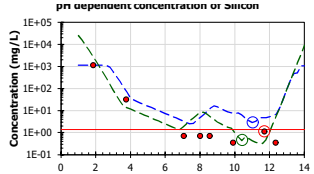
pH dependent concentration of Potassium



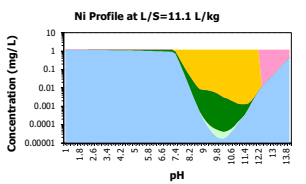
pH dependent concentration of Selenium



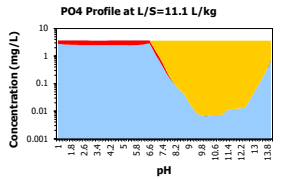
pH dependent concentration of Silicon



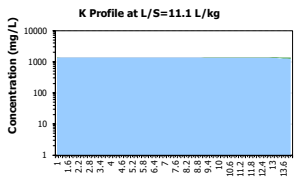
Ni Profile at L/S=11.1 L/kg



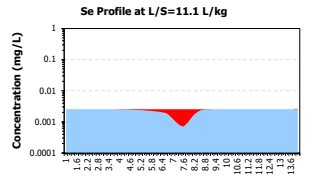
PO4 Profile at L/S=11.1 L/kg



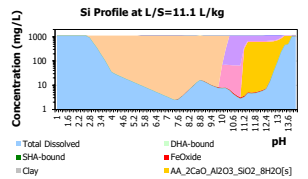
K Profile at L/S=11.1 L/kg



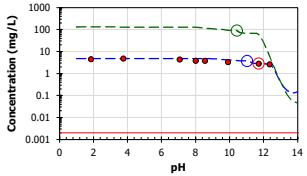
Se Profile at L/S=11.1 L/kg



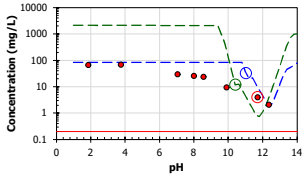
Si Profile at L/S=11.1 L/kg



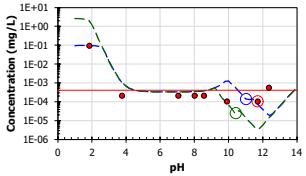
pH dependent concentration of Strontium



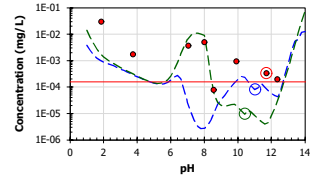
pH dependent concentration of Sulfate



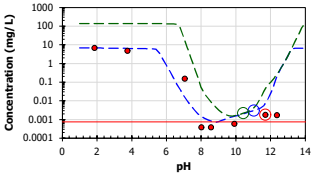
pH dependent concentration of Tin



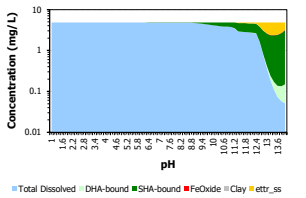
pH dependent concentration of Vanadium



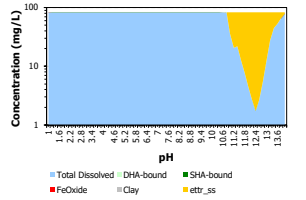
pH dependent concentration of Zinc



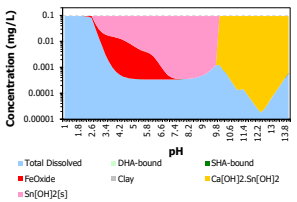
Sr Profile at L/S=11.1 L/kg



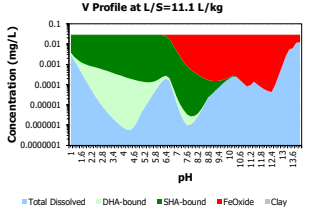
SO4 Profile at L/S=11.1 L/kg



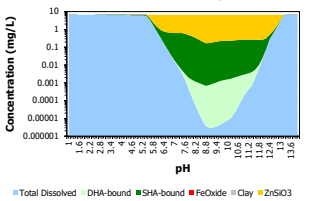
Sn Profile at L/S=11.1 L/kg



V Profile at L/S=11.1 L/kg



Zn Profile at L/S=11.1 L/kg



Model Comparison: residuals - Concentration

Sample

Name Industrial CN site

Legend

Total Average Deviation Square root of the sum of the squared values of residuals divided by the number of values, over the entire X range.
User Average Deviation Square root of the sum of the squared values of residuals divided by the number of values, over the user defined X range.
Fractional Average Deviation Square root of the sum of the squared values of residuals divided by the number of values, over the fraction.
Note that the Total and User Average Deviation columns are averages as well.

Residual details, concentrations

Residuals as log(model/sample)

Fraction	*8*	*7*	*6*	*5*	*4*	*3*	*2*	*1*	*Total Avg*
pH	*1.85*	*3.75*	*7.05*	*8.00*	*8.55*	*9.90*	*11.7*	*12.4*	*Deviation*
Al	0.00	0.01	-1.87	-2.11	-2.38	0.10	-0.31	0.45	0.47
As	-0.12	1.27	-1.08	-1.46	-0.57	0.02	0.64	0.51	0.30
Ba	0.01	0.00	0.12	0.18	0.20	0.15	0.13	0.15	0.05
Br	0.27	0.28	0.05	0.04	0.00	0.02	0.10	0.10	0.05
Ca	0.03	0.00	0.01	0.07	0.10	-0.04	-0.32	-0.22	0.05
Cd	0.00	0.11	-0.31	0.48	0.32	0.13	0.54	0.30	0.11
Cl	-0.01	-0.04	-0.05	-0.04	-0.04	-0.02	0.00	0.00	0.01
CNT	0.12	0.27	0.02	0.29	0.16	1.06	0.83	-0.33	0.18
Co	0.00	-0.01	0.09	1.67	2.13	-0.52	0.57	1.11	0.38
CO32-	-	-	-	-	-	-	-	-	-
Cr	-1.54	-1.10	0.81	0.86	0.93	0.92	-0.20	0.53	0.33
Cu	-0.18	-0.51	2.09	1.97	0.59	1.73	0.80	1.05	0.46
F	0.00	0.05	-1.54	-0.89	-0.94	-0.31	-0.70	-0.69	0.28
Fe	-0.03	0.38	0.48	0.39	0.12	0.64	-0.01	0.38	0.13
B	0.00	0.09	0.38	0.55	1.78	2.08	1.13	-1.04	0.40
Si	0.00	0.36	0.67	0.84	1.22	1.35	0.62	1.29	0.32
K	0.01	-0.01	0.00	-0.04	0.02	0.00	-0.01	0.00	0.01
Li	0.01	0.00	0.07	0.12	0.08	0.27	0.01	-0.10	0.04
Mg	0.00	0.00	0.04	0.06	0.15	-1.22	-0.82	-1.27	0.24
Mn	0.00	0.00	0.14	0.56	2.58	3.94	0.91	0.55	0.61
Mo	0.69	1.89	0.17	0.04	0.00	0.55	0.11	-0.47	0.27
Na	0.03	-0.07	-0.07	-0.07	-0.07	-0.09	-0.01	-0.19	0.03
Ni	-0.01	0.05	0.26	0.54	0.65	-1.27	-0.11	1.73	0.29
Pb	-0.04	0.24	1.07	0.73	0.70	0.12	0.88	1.18	0.26
PO4	-	-	-	-	-	-	-	-	-
Sb	0.00	0.42	0.44	0.43	0.18	1.25	1.21	-0.48	0.25
Se	0.57	0.56	0.22	0.27	0.52	0.13	0.24	0.00	0.13
Sn	-0.01	0.72	0.21	0.22	0.26	1.07	-0.15	-1.45	0.25
SO4	0.09	0.08	0.44	0.51	0.54	0.94	0.39	-0.03	0.17
Sr	0.02	0.00	0.04	0.09	0.10	0.09	0.00	0.00	0.02
V	-1.47	-0.78	-2.24	-3.26	-0.91	-0.75	-0.59	-0.66	0.57
W	-1.10	0.63	0.67	0.67	0.67	1.18	0.70	1.10	0.31
Zn	0.00	0.13	-0.99	0.58	0.34	0.39	0.62	2.05	0.31
Avg Deviation	0.08	0.10	0.15	0.18	0.17	0.20	0.10	0.15	0.24

Yellow = own pH All residuals within + 1 or - 1 are considered to represent a good fit. 0 of coarse the best.

B	Phase missing pH 8-12
Sb	Actually pretty good description for a difficult element
CN	Note description of CN with ettringite substitution!!!