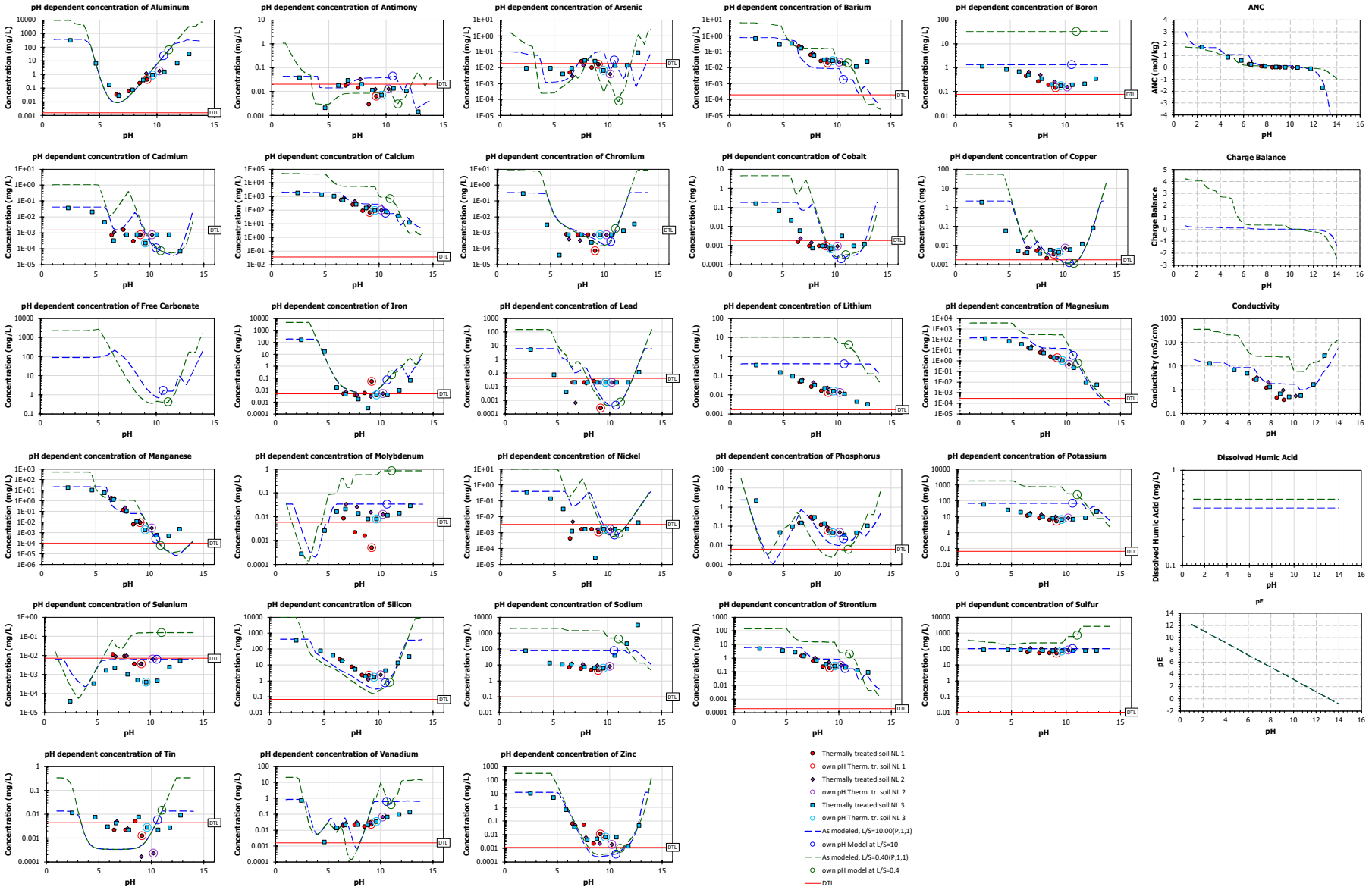
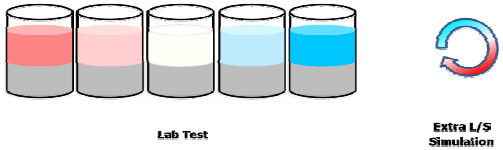

pH dependent concentration of Aluminum
pH dependent concentration of Antimony
pH dependent concentration of Arsenic
pH dependent concentration of Barium
pH dependent concentration of Boron
ANC
pH dependent concentration of Cadmium
pH dependent concentration of Calcium
pH dependent concentration of Chromium
pH dependent concentration of Cobalt
pH dependent concentration of Copper
Charge Balance
pH dependent concentration of Free Carbonate
pH dependent concentration of Iron
pH dependent concentration of Lead
pH dependent concentration of Lithium
pH dependent concentration of Magnesium
Conductivity
pH dependent concentration of Manganese
pH dependent concentration of Molybdenum
pH dependent concentration of Nickel
pH dependent concentration of Phosphorus
pH dependent concentration of Potassium
Dissolved Humic Acid
pH dependent concentration of Selenium
pH dependent concentration of Silicon
pH dependent concentration of Sodium
pH dependent concentration of Strontium
pH dependent concentration of Sulfur
pE
pH dependent concentration of Tin
pH dependent concentration of Vanadium
pH dependent concentration of Zinc
Concentration (mg/L)
ANC (mol/kg)
Charge Balance
Conductivity (mS/cm)
Dissolved Humic Acid (mg/L)
pE
pH
DTL
Thermally treated soil NL 1
own pH Therm. tr. soil NL 1
Thermally treated soil NL 2
own pH Therm. tr. soil NL 2
Thermally treated soil NL 3
own pH Therm. tr. soil NL 3
As modeled, L/S=10.00(P,1,1)
own pH Model at L/S=10
As modeled, L/S=0.40(P,1,1)
own pH model at L/S=0.4
DTL

Object pH Dependent Leaching Test Model
Name Thermally treated soil NL

pH Dependent Leaching Test Scenario



Lab Test

Model Parameters

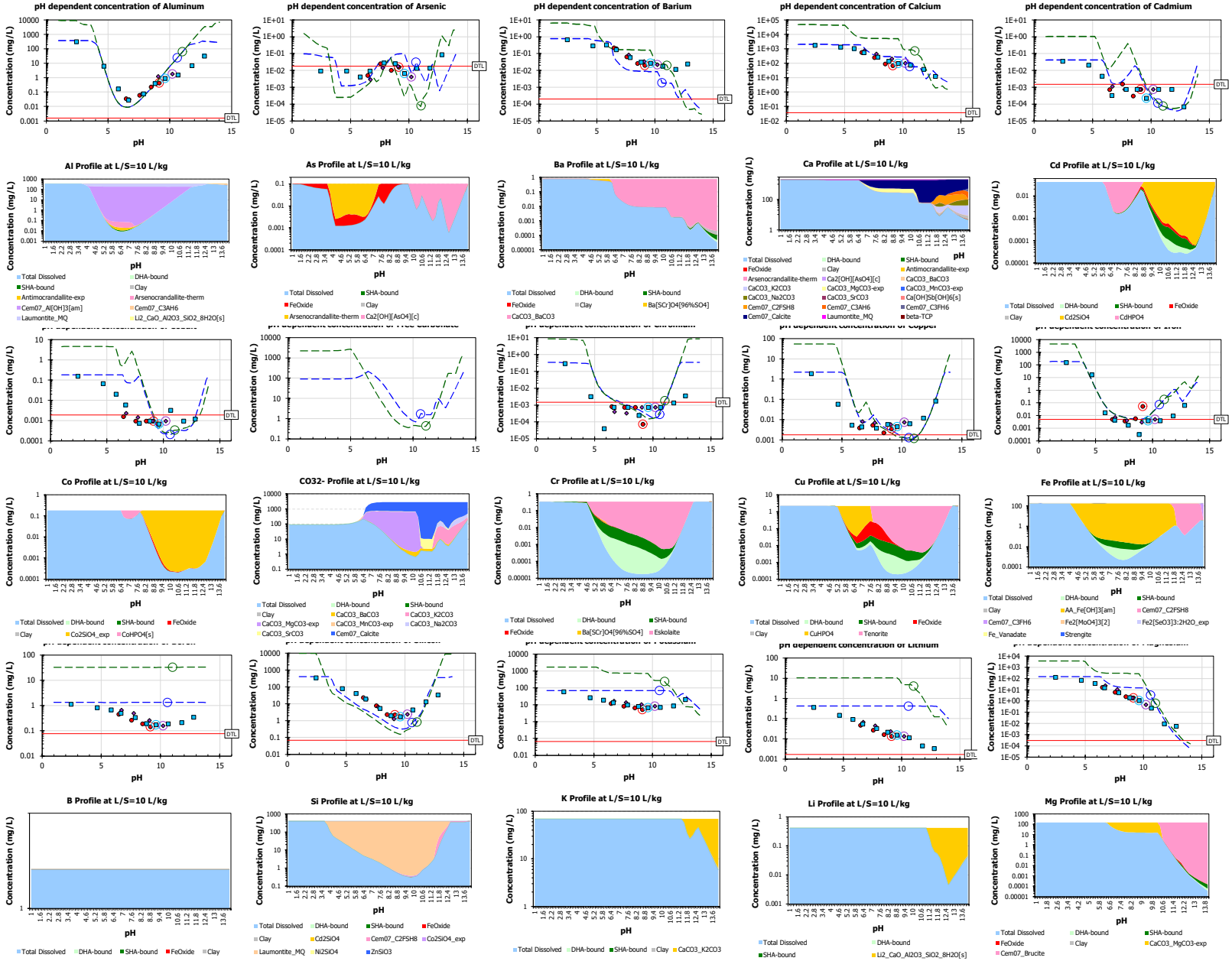
Entity	Unit	Default
c0		-6.699
c1		3.144E-11
c2		-9.796E-12
c3		1.397E-12
c4		-9.302E-14
c5		2.346E-15
Clay	mg/kg	8000
Hydrous Ferric Oxide	mg/kg	70.00
L/S	L/kg	10.00
pE		7.300
pH		5.860
Solid Humic Acid	mg/kg	20.00
Simulated Low L/S	L/kg	0.4000

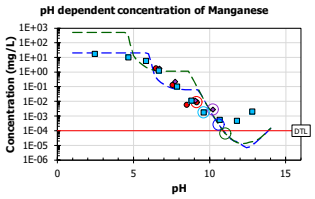
Available Content

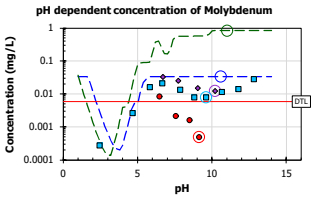
Entity	mg/kg	Entity	mg/kg	Entity	mg/kg
Acetic acid	2.220E-08	F	1.900E-09	Pb	61.18
Ag	1.079E-08	Fe	1859	PO4	79.50
Al	3739	B	13.31	Sb	0.4414
As	1.030	Si	4070	Se	0.06251
Ba	7.838	Hg	2.006E-08	Sn	0.1347
Br	7.990E-09	K	696.2	SO4	3186
Ca	2.065E+04	Li	4.203	Sr	59.88
Cd	0.4203	Mg	1485	Th	2.320E-08
Cl	100.0	Mn	204.0	U	2.380E-08
Co	1.817	Mo	0.3366	V	8.431
CO32-	2.785E+04	Na	800.0	Zn	125.0
Cr	3.440	Ni	3.861		
Cu	22.02	NO3	6.200E-09		

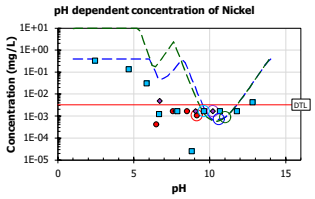
Minerals

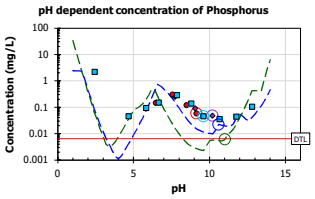
Name	Log(K)	Reaction
AA_Fe[OH]3[am]	16.60	AA_Fe[OH]3[am] + 1 H2O -> 1 Fe[OH]4- + 1 H+
Antimocrandallite-exp	63.00	Antimocrandallite-exp + 8 H2O -> 3 Al[OH]4- + 1 Ca+2 + 3 H+ + 2 Sb[OH]6-
Arsenocrandallite-ther	95.56	Arsenocrandallite-therm + 6 H2O -> 3 Al[OH]4- + 2 AsO4-3 + 1 Ca+2 + 7 H+
Ba[SCr]O4[96%SO4]	9.790	Ba[SCr]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2
BaSrSO4[50%Ba]	8.221	BaSrSO4[50%Ba] -> 0.5 Ba+2 + 1 SO4-2 + 0.5 Sr+2
beta-TCP	28.93	beta-TCP -> 3 Ca+2 + 2 PO4-3
Ca[OH]Sb[OH]6[s]	2.000	Ca[OH]Sb[OH]6[s] + 1 H+ -> 1 Ca+2 + 1 H2O + 1 Sb[OH]6-
Ca2[OH][AsO4][c]	4.000	Ca2[OH][AsO4][c] + 1 H+ -> 1 AsO4-3 + 2 Ca+2 + 1 H2O
Ca5[OH][VO4]3[c]	-61.00	Ca5[OH][VO4]3[c] + 13 H+ -> 5 Ca+2 + 7 H2O + 3 VO2+
CaCO3_BaCO3	22.00	CaCO3_BaCO3 -> 1 Ba+2 + 2 CO3-2 + 1 Ca+2
CaCO3_K2CO3	19.30	CaCO3_K2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 K+
CaCO3_Li2CO3	21.30	CaCO3_Li2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 Li+
CaCO3_MgCO3-exp	18.02	CaCO3_MgCO3-exp -> 2 CO3-2 + 1 Ca+2 + 1 Mg+2
CaCO3_MnCO3-exp	20.78	CaCO3_MnCO3-exp -> 2 CO3-2 + 1 Ca+2 + 1 Mn+2
CaCO3_Na2CO3	18.30	CaCO3_Na2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 Na+
CaCO3_SrCO3	19.85	CaCO3_SrCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Sr+2
CaMoO4[s]	7.950	CaMoO4[s] -> 1 Ca+2 + 1 MoO4-2
CaSb[OH]6[s]2_exp	19.41	CaSb[OH]6[s]2_exp -> 1 Ca+2 + 2 Sb[OH]6-
Cd2SiO4	6.059	Cd2SiO4 + 2 H+ -> 2 Cd+2 + 1 H2SiO4-2
CdHPO4	26.48	CdHPO4 -> 1 Cd+2 + 1 H+ + 1 PO4-3
Cem07_Al[OH]3[am]	13.76	Cem07_Al[OH]3[am] + 1 H2O -> 1 Al[OH]4- + 1 H+
Cem07_Brucite	-16.83	Cem07_Brucite + 2 H+ -> 2 H2O + 1 Mg+2
Cem07_C2FSH8	21.41	Cem07_C2FSH8 -> 2 Ca+2 + 2 Fe[OH]4- + 3 H2O + 1 H2SiO4-2
Cem07_C3AH6	-35.14	Cem07_C3AH6 + 4 H+ -> 2 Al[OH]4- + 3 Ca+2 + 4 H2O
Cem07_C3FH6	-30.82	Cem07_C3FH6 + 4 H+ -> 3 Ca+2 + 2 Fe[OH]4- + 4 H2O
Cem07_CAH10	7.505	Cem07_CAH10 -> 2 Al[OH]4- + 1 Ca+2 + 6 H2O
Cem07_Calcite	8.485	Cem07_Calcite -> 1 CO3-2 + 1 Ca+2
Cem07_Gypsum	4.583	Cem07_Gypsum -> 1 Ca+2 + 2 H2O + 1 SO4-2
Cerrusite	13.13	Cerrusite -> 1 CO3-2 + 1 Pb+2
Co2SiO4_exp	6.469	Co2SiO4_exp + 2 H+ -> 2 Co+2 + 1 H2SiO4-2
CoHPO4[s]	24.48	CoHPO4[s] -> 1 Co+2 + 1 H+ + 1 PO4-3
CuHPO4	26.00	CuHPO4 -> 1 Cu+2 + 1 H+ + 1 PO4-3
Eskolaite	139.5	Eskolaite + 5 H2O -> 2 CrO4-2 + 10 H+ + 6 e-
Fe_Vanadate	19.18	Fe_Vanadate + 1 H2O -> 0.5 Fe[OH]4- + 1 VO2+ + 0.5 e-
Fe2[MoO4]3[2]	86.35	Fe2[MoO4]3[2] + 8 H2O -> 2 Fe[OH]4- + 8 H+ + 3 MoO4-2
Fe2[SeO3]3:2H2O_exp	180.0	Fe2[SeO3]3:2H2O_exp + 7 H2O -> 2 Fe[OH]4- + 14 H+ + 3 SeO4-2 + 6 e-
Laumontite_MQ	118.0	Laumontite_MQ + 8 H2O -> 2 Al[OH]4- + 1 Ca+2 + 8 H+ + 4 H2SiO4-2
Manganite	-25.27	Manganite + 3 H+ + 1 e- -> 2 H2O + 1 Mn+2
Ni[OH]2[s]	-10.80	Ni[OH]2[s] + 2 H+ -> 2 H2O + 1 Ni+2
Ni2SiO4	5.498	Ni2SiO4 + 2 H+ -> 1 H2SiO4-2 + 2 Ni+2
NiHPO4	25.00	NiHPO4 -> 1 H+ + 1 Ni+2 + 1 PO4-3
Pb[OH]2[C]	-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
Pb3[VO4]2	-6.357	Pb3[VO4]2 + 8 H+ -> 4 H2O + 3 Pb+2 + 2 VO2+
PbHPO4-wf2	25.48	PbHPO4-wf2 -> 1 H+ + 1 PO4-3 + 1 Pb+2
PbMoO4[cc]	13.36	PbMoO4[cc] -> 1 MoO4-2 + 1 Pb+2
Sn[OH]2[s]	1.447	Sn[OH]2[s] + 2 H+ -> 2 H2O + 1 Sn+2
Strengite	48.00	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
Tenorite	-7.620	Tenorite + 2 H+ -> 1 Cu+2 + 1 H2O
ZnSiO3	18.69	ZnSiO3 + 1 H2O -> 1 H2SiO4-2 + 1 Zn+2

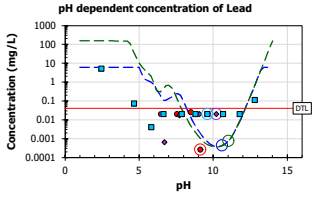

pH dependent concentration of Aluminum
pH dependent concentration of Arsenic
pH dependent concentration of Barium
pH dependent concentration of Calcium
pH dependent concentration of Cadmium
Al Profile at L/S=10 L/kg
As Profile at L/S=10 L/kg
Ba Profile at L/S=10 L/kg
Ca Profile at L/S=10 L/kg
Cd Profile at L/S=10 L/kg
Co Profile at L/S=10 L/kg
CO32- Profile at L/S=10 L/kg
Cr Profile at L/S=10 L/kg
Cu Profile at L/S=10 L/kg
Fe Profile at L/S=10 L/kg
B Profile at L/S=10 L/kg
Si Profile at L/S=10 L/kg
K Profile at L/S=10 L/kg
Li Profile at L/S=10 L/kg
Mg Profile at L/S=10 L/kg
Concentration (mg/L)
pH
DTL
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Antimocrandallite-exp
Arsenocrandallite-therm
Ca2[OH][AsO4][c]
CaCO3_BaCO3
CaCO3_K2CO3
CaCO3_MgCO3-exp
CaCO3_MnCO3-exp
CaCO3_Na2CO3
CaCO3_SrCO3
Ca[OH]Sb[OH]6[s]
Cem07_C2FSH8
Cem07_C3AH6
Cem07_C3FH6
Cem07_Calcite
Laumontite_MQ
beta-TCP
Cem07_Al[OH]3[am]
Li2_CaO_Al2O3_SiO2_8H2O[s]
Ba[SCr]O4[96%SO4]
CaCO3_BaCO3
Cd2SiO4
CdHPO4
Co2SiO4_exp
CoHPO4[s]
CaCO3_K2CO3
Cem07_Calcite
Eskolaite
AA_Fe[OH]3[am]
Cem07_C2FSH8
Cem07_C3FH6
Fe2[MoO4]3[2]
Fe2[SeO3]3:2H2O_exp
Fe_Vanadate
Strengite
CuHPO4
Tenorite
Si
Cd2SiO4
Cem07_C2FSH8
Co2SiO4_exp
Laumontite_MQ
Ni2SiO4
ZnSiO3
K
CaCO3_K2CO3
Li
Li2_CaO_Al2O3_SiO2_8H2O[s]
Mg
Cem07_Brucite

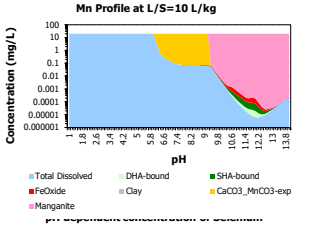

pH dependent concentration of Manganese
Concentration (mg/L)
pH
DTL

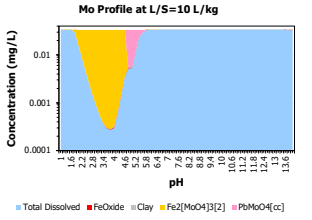

pH dependent concentration of Molybdenum
Concentration (mg/L)
pH
DTL

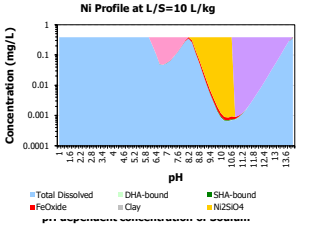

pH dependent concentration of Nickel
Concentration (mg/L)
pH
DTL

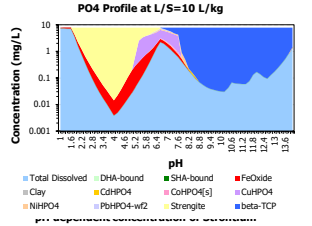

pH dependent concentration of Phosphorus
Concentration (mg/L)
pH
DTL

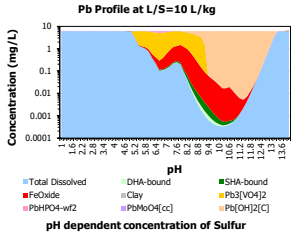

pH dependent concentration of Lead
Concentration (mg/L)
pH
DTL

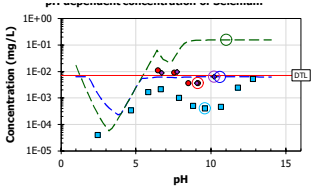

Mn Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
CaCO3_MnCO3-exp
Manganite

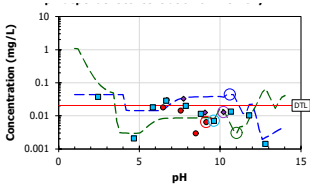

Mo Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
FeOxide
Clay
Fe2[MoO4]3[2]
PbMoO4[cc]

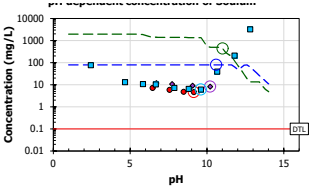

Ni Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Ni2SiO4

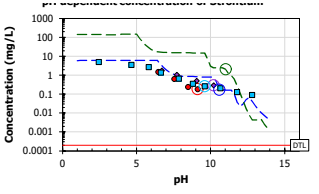

PO4 Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
CdHPO4
CoHPO4[s]
CuHPO4
NiHPO4
PbHPO4-wf2
Strengite
beta-TCP

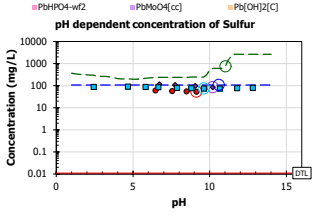

Pb Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Pb3[VO4]2
PbHPO4-wf2
PbMoO4[cc]
Pb[OH]2[C]

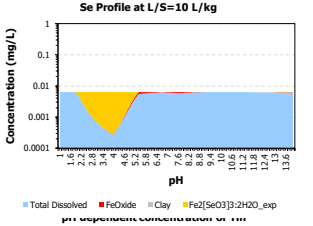

Concentration (mg/L)
pH
DTL

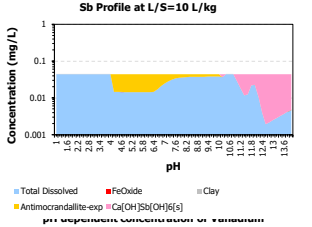

Concentration (mg/L)
pH
DTL

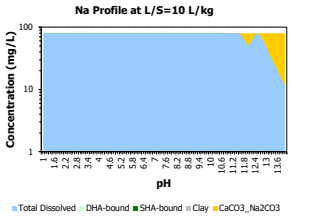

Concentration (mg/L)
pH
DTL

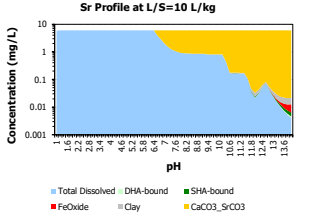

Concentration (mg/L)
pH
DTL

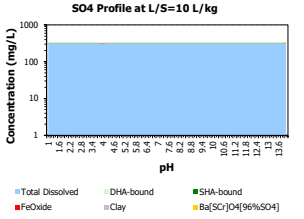

pH dependent concentration of Sulfur
Concentration (mg/L)
pH
DTL

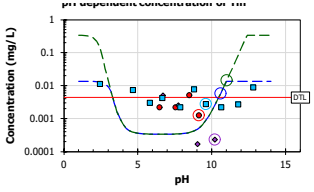

Se Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
FeOxide
Clay
Fe2[SeO3]3:2H2O_exp

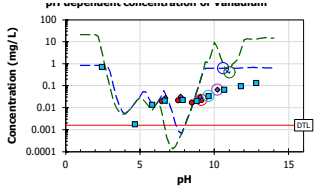

Sb Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
FeOxide
Clay
Antimocrandallite-exp
Ca[OH]Sb[OH]6[s]

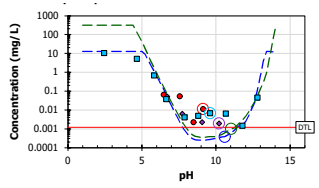

Na Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
Clay
CaCO3_Na2CO3

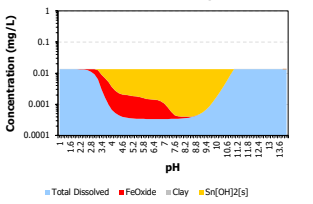

Sr Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
CaCO3_SrCO3

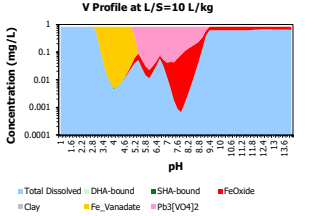

SO4 Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Ba[SCr]O4[96%SO4]

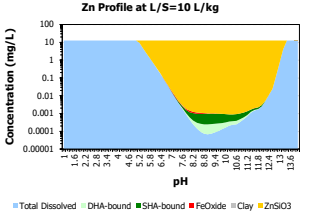

Concentration (mg/L)
pH
DTL


Concentration (mg/L)
pH
DTL


Concentration (mg/L)
pH
DTL


Sn Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
FeOxide
Clay
Sn[OH]2[s]


V Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Fe_Vanadate
Pb3[VO4]2


Zn Profile at L/S=10 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ZnSiO3

Model Comparison: residuals - Concentration

Name Thermally treated soil NL

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	*10*	*9*	*8*	*7*	*6*	*5*	*4*	*3*	*2*	*1*	*Total Avg*
pH	*2.44*	*4.66*	*5.82*	*6.65*	*7.86*	*8.80*	*9.60*	*10.7*	*11.8*	*12.8*	*Deviation*
Al	0.07	-0.02	-0.96	-0.48	-0.18	-0.01	0.43	1.24	1.47	1.03	0.25
As	0.90	-0.87	-0.43	-0.35	-0.29	0.54	1.18	0.28	-0.05	-1.84	0.27
B	0.07	0.21	0.29	0.42	0.59	0.83	0.88	0.85	0.80	0.59	0.20
Ba	0.07	0.36	0.20	-0.63	-0.77	-0.53	-0.50	-1.01	-1.44	-1.76	0.28
Ca	0.07	0.16	0.27	0.35	0.08	0.32	0.46	-0.11	-0.43	0.21	0.09
Cd	0.07	0.30	0.94	0.76	0.72	1.30	0.58	-0.85	-1.21	0.13	0.25
Cl	-	-	-	-	-	-	-	-	-	-	-
Co	0.07	0.43	0.95	1.16	2.26	0.65	-0.29	-1.18	-0.48	0.06	0.31
CO32-	-	-	-	-	-	-	-	-	-	-	-
Cr	0.06	1.83	2.11	0.46	0.10	0.32	-0.47	-0.36	1.35	1.99	0.38
Cu	0.07	1.57	1.36	0.21	0.46	-0.23	-0.35	-0.69	-0.49	0.09	0.23
F	-	-	-	-	-	-	-	-	-	-	-
Fe	0.06	-0.44	0.58	0.48	0.55	1.20	0.38	1.33	2.06	0.54	0.30
K	0.07	0.42	0.57	0.72	0.85	0.94	1.02	1.00	0.64	0.23	0.23
Li	0.07	0.46	0.66	0.89	1.11	1.29	1.43	1.57	1.97	2.10	0.41
Mg	0.07	0.32	0.60	0.64	0.50	0.89	1.13	1.05	0.35	-0.89	0.23
Mn	0.07	0.31	0.54	-0.68	-0.17	0.74	0.89	-0.41	-1.43	-2.30	0.31
Mo	1.04	0.18	0.31	0.20	0.39	0.62	0.62	0.47	0.38	0.07	0.16
Na	0.01	0.79	0.87	0.88	1.04	1.10	1.11	0.30	-0.51	-1.70	0.30
Ni	0.07	0.46	1.10	1.59	2.10	3.32	0.19	-0.36	0.30	0.85	0.45
Pb	0.07	1.92	2.38	0.72	0.89	-0.63	-1.47	-1.65	-0.40	0.76	0.41
PO4	-	-	-	-	-	-	-	-	-	-	-
Sb	0.07	0.85	-0.10	-0.21	0.25	0.51	0.74	0.51	0.30	0.19	0.14
Se	1.56	0.53	0.54	0.45	0.76	1.10	1.19	1.13	0.41	0.07	0.28
Si	0.07	-0.34	-0.63	-0.66	-0.57	-0.55	-0.72	-0.73	0.07	1.03	0.19
Sn	0.05	-1.28	-0.95	-1.10	-0.80	-1.26	-0.50	0.47	0.69	0.18	0.26
SO4	-	-	-	-	-	-	-	-	-	-	-
Sr	0.07	0.22	0.34	0.42	0.15	0.38	0.49	-0.09	-0.52	-0.34	0.11
V	0.07	0.96	0.02	0.38	-1.43	0.37	1.26	0.97	0.82	0.70	0.26
Zn	0.07	0.37	0.22	0.22	-0.66	-1.31	-1.38	-1.22	0.08	0.44	0.24
Avg Deviation	0.08	0.16	0.18	0.14	0.18	0.21	0.18	0.18	0.19	0.21	0.26

Yellow = own pH All residuals within + 1 or - 1 are considered to represent a good fit.

As	Measurements at MDL
K	Both Na and K show similar pH dependence, which may be linked to dissolution of silica phases. Otherwise no indication what is causing this behaviour
Li	Strong pH dependent behaviour. As yet no phases identified that can explain the behaviour over the wide pH range where solibility control is active. Possibly linked to Si phases?
Mg	Further look into carbonate phases
Na	Both Na and K show similar pH dependence, which may be linked to dissolution of silica phases. Otherwise no indication what is causing this behaviour
Pb	Measurements at MDL
Se	Difficult element to capture due to lacking thermodynamic data. Experimental minerals may need to be adjusted.
V	Reasonable description. Info lacking at pH > 9
Zn	Good description. Measurements at own pH at MDL