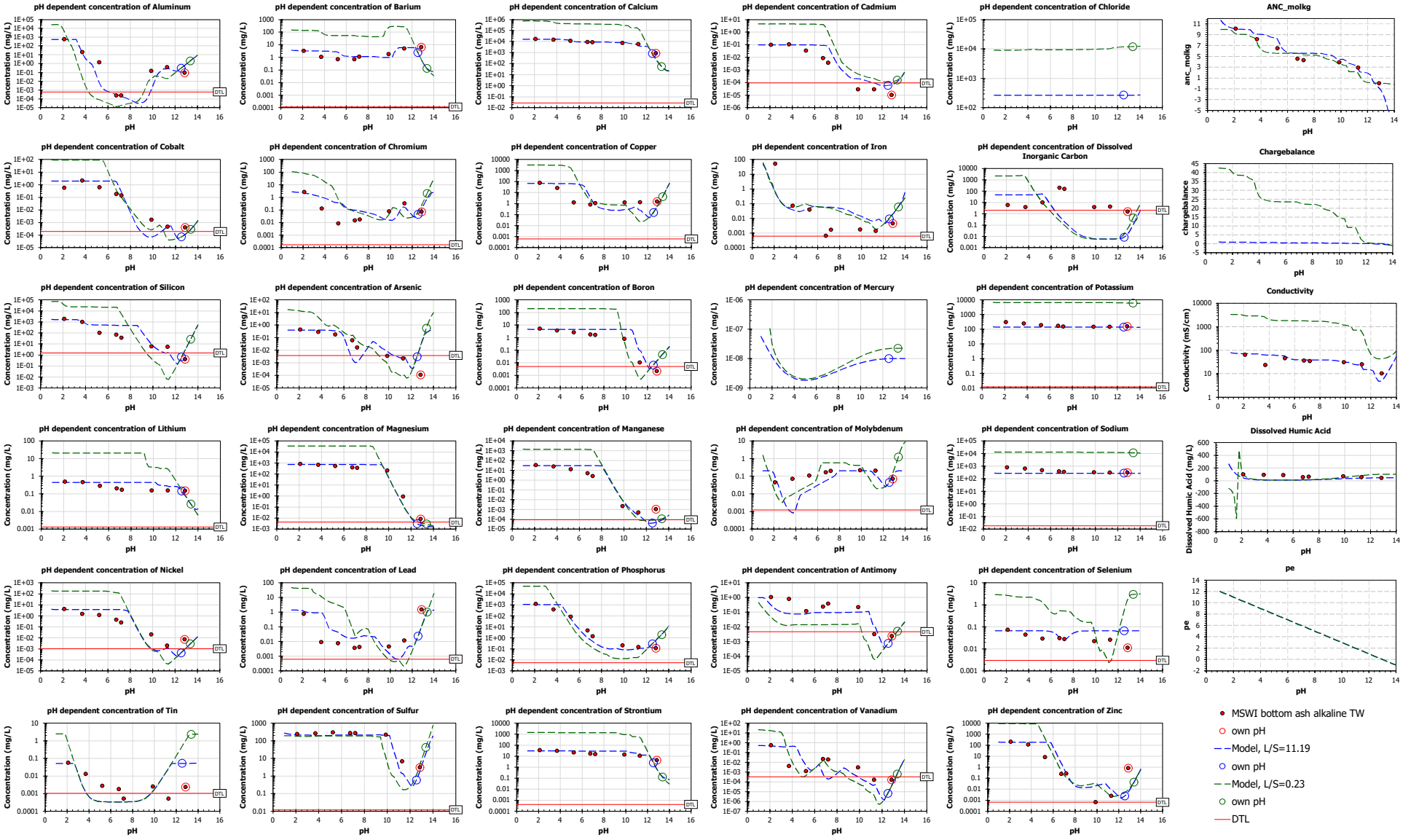
COMPARISON pH DEPENDENCE DATA WITH MODEL



Name MSWI BA TW Alkaline

pH Dependent Leaching Test Scenario

Lab Test

Extra L/S Simulation

Chemical

Model Parameters

Entity	Unit	Default
c0		-2.448
c1		-1.501
c2		0.2591
c3		-0.01717
c4		0.0003948
c5		2.043E-08
Clay	mg/kg	2.000E+04
Dissolved Humic Ac	mg/L	20.40
Hydrous Ferric Oxid	mg/kg	1900
L/S	L/kg	11.19
pe		1.000
pH		12.00
Solid Humic Acid	mg/kg	916.1
Extra L/S	L/kg	0.2343

Available Content

Entity	Unit	Default	Entity	Unit	Default	Entity	Unit	Default
Ac	mg/kg	2.270E-07	As	mg/kg	4.419	Sn	mg/kg	0.5849
Ag	mg/kg	1.079E-07	B	mg/kg	51.71	S	mg/kg	3060
Al	mg/kg	6036	Hg	mg/kg	2.006E-07	Sr	mg/kg	355.6
Ba	mg/kg	65.30	K	mg/kg	1592	Th	mg/kg	2.320E-07
Br	mg/kg	2.000	Li	mg/kg	4.982	U	mg/kg	2.380E-07
Ca	mg/kg	1.794E+05	Mg	mg/kg	8123	V	mg/kg	5.542
Cd	mg/kg	1.085	Mn	mg/kg	341.6	Zn	mg/kg	2114
Cl	mg/kg	3000	Mo	mg/kg	2.262			
Co	mg/kg	21.86	Na	mg/kg	3076			
Cr	mg/kg	27.10	Ni	mg/kg	42.28			
Cu	mg/kg	761.3	NO3	mg/kg	200.0			
F	mg/kg	15.00	Pb	mg/kg	15.39			
Fe	mg/kg	519.8	P	mg/kg	1.232E+04			
CO32-	mg/kg	8.110E+04	Sb	mg/kg	10.87			
Si	mg/kg	1.864E+04	Se	mg/kg	0.7485			

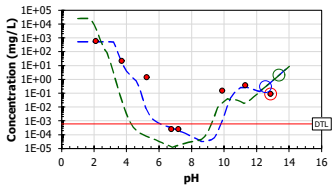
Solid Solutions

Name	End Member	Log(K)	Reaction
ettr_ss	AsO4_Ettringite_ss	-35.00	AsO4_Ettringite_ss + 10 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 H3AsO4 + 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	-74.59	BO3_Ettringite_ss + 10 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 H3BO3 + 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
	Fe_Ettringite_ss	-8.000	Fe_Ettringite_ss + 4 H+ + 8 H2O -> 6 Ca+2 + 2 Fe[OH]4- + 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
	PO4_Ettringite_ss	39.10	PO4_Ettringite_ss + 1 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 PO4-3 + 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	-8.592	SeO4-2_Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 SeO4-2 + 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

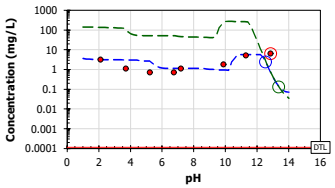
Minerals

Name	> 1E-13 mol/kg	Log(K)	Reaction
AA_Brucite	Yes	-16.84	AA_Brucite + 2 H+ -> 2 H2O + 1 Mg+2
AA_Calcite	Yes	-7.200	AA_Calcite + 2 H+ -> 1 Ca+2 + 1 H2CO3
AA_Fe[OH]3[microc	Yes	18.60	AA_Fe[OH]3[microcr] + 1 H2O -> 1 Fe[OH]4- + 1 H+
AA_Gypsum	Yes	4.600	AA_Gypsum -> 1 Ca+2 + 2 H2O + 1 SO4-2
AA_Jennite	Yes	-7.026	AA_Jennite + 1.2 H+ -> 1.5 Ca+2 + 2.1 H2O + 0.9 H2SiO4-2
AA_Portlandite	Yes	-22.80	AA_Portlandite + 2 H+ -> 1 Ca+2 + 2 H2O
AA_Tobermorite-II	Yes	17.89	AA_Tobermorite-II -> 1.5 Ca+2 + 0.6 H+ + 0.9 H2O + 1.8 H2SiO4-2
alpha-TCP	Yes	25.50	alpha-TCP -> 3 Ca+2 + 2 PO4-3
Ba[SCr]O4[77%SO4	Yes	10.13	Ba[SCr]O4[77%SO4] -> 1 Ba+2 + 0.23 CrO4-2 + 0.77 SO4-2
BaSrSO4[50%Ba]	Yes	8.221	BaSrSO4[50%Ba] -> 0.5 Ba+2 + 1 SO4-2 + 0.5 Sr+2
Ca[OH]2.Co[OH]2	Yes	-32.40	Ca[OH]2.Co[OH]2 + 4 H+ -> 1 Ca+2 + 1 Co+2 + 4 H2O
Ca[OH]2.Cu[OH]2	Yes	-31.00	Ca[OH]2.Cu[OH]2 + 4 H+ -> 1 Ca+2 + 1 Cu+2 + 4 H2O
Ca[OH]2.Ni[OH]2	Yes	-32.00	Ca[OH]2.Ni[OH]2 + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Ni+2
Ca[OH]2.Pb[OH]2	Yes	-30.00	Ca[OH]2.Pb[OH]2 + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Pb+2
Ca[OH]2.Zn[OH]2	Yes	-30.52	Ca[OH]2.Zn[OH]2 + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Zn+2
Ca3[AsO4]2:6H2O	Yes	-22.30	Ca3[AsO4]2:6H2O + 6 H+ -> 3 Ca+2 + 6 H2O + 2 H3AsO4
Ca4Cd[PO4]3OH	Yes	39.23	Ca4Cd[PO4]3OH + 1 H+ -> 4 Ca+2 + 1 Cd+2 + 1 H2O + 3 PO4-3
CaMoO4[c]	Yes	7.940	CaMoO4[c] -> 1 Ca+2 + 1 MoO4-2
CaPb2[PO4]2	Yes	40.76	CaPb2[PO4]2 -> 1 Ca+2 + 2 PO4-3 + 2 Pb+2
CaSb[OH]6[s]2	Yes	19.41	CaSb[OH]6[s]2 + 6 H2O -> 1 Ca+2 + 2 Sb[OH]6-
CaSeO3:2H2O	Yes	33.51	CaSeO3:2H2O -> 1 Ca+2 + 2 H+ + 1 H2O + 1 SeO4-2 + 2 e-
CoSiO4	Yes	6.289	CoSiO4 + 2 H+ -> 2 Co+2 + 1 H2SiO4-2
Cr[OH]3[A]	Yes	68.13	Cr[OH]3[A] + 1 H2O -> 1 CrO4-2 + 5 H+ + 3 e-
Cu2SiO4	Yes	6.059	Cu2SiO4 + 2 H+ -> 2 Cu+2 + 1 H2SiO4-2
Diaspore	Yes	16.13	Diaspore + 2 H2O -> 1 Al[OH]4- + 1 H+
Fe_Vanadaat	Yes	24.98	Fe_Vanadaat + 2 H2O -> 1 Fe[OH]4- + 1 VO2+
Fluorite	Yes	10.96	Fluorite -> 1 Ca+2 + 2 F-
Laumontite	Yes	118.0	Laumontite + 8 H2O -> 2 Al[OH]4- + 1 Ca+2 + 8 H+ + 4 H2SiO4-2
Manganite	Yes	-25.27	Manganite + 3 H+ + 1 e- -> 2 H2O + 1 Mn+2
Ni[OH]2[s]	Yes	-10.80	Ni[OH]2[s] + 2 H+ -> 2 H2O + 1 Ni+2
OCP	Yes	46.90	OCP -> 4 Ca+2 + 1 H+ + 2.5 H2O + 3 PO4-3
Pb[OH]2[C]	Yes	-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
Pb2V2O7	Yes	0.9500	Pb2V2O7 + 3 H+ -> 1.5 H2O + 1 Pb+2 + 1 VO2+
Pb3[VO4]2	Yes	-3.070	Pb3[VO4]2 + 4 H+ -> 2 H2O + 1.5 Pb+2 + 1 VO2+
PbMoO4[c]	Yes	15.80	PbMoO4[c] -> 1 MoO4-2 + 1 Pb+2
Sn[OH]2[s]	Yes	1.447	Sn[OH]2[s] + 2 H+ -> 2 H2O + 1 Sn+2
Strengite	Yes	48.00	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
Willemite	Yes	6.289	Willemite + 2 H+ -> 1 H2SiO4-2 + 2 Zn+2

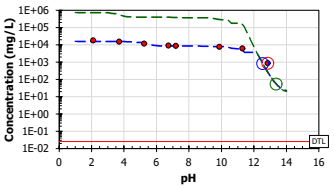
pH dependent concentration of Aluminum



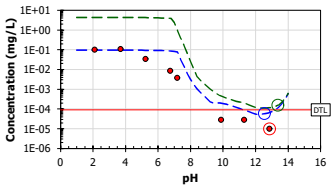
pH dependent concentration of Barium



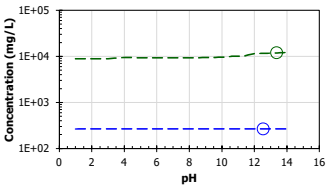
pH dependent concentration of Calcium



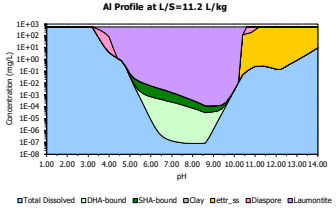
pH dependent concentration of Cadmium



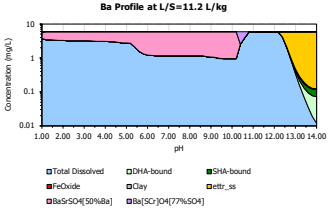
pH dependent concentration of Chloride



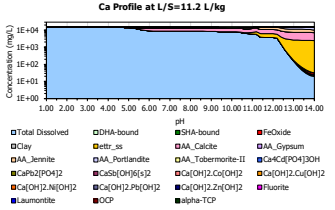
Al Profile at L/S=11.2 L/kg



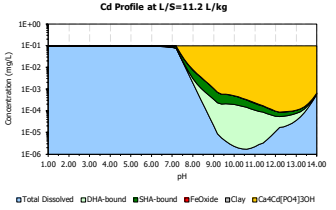
Ba Profile at L/S=11.2 L/kg



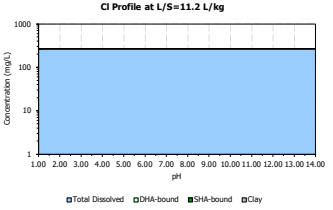
Ca Profile at L/S=11.2 L/kg



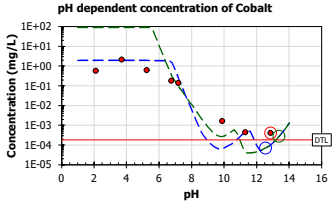
Cd Profile at L/S=11.2 L/kg



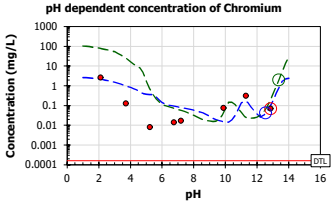
Cl Profile at L/S=11.2 L/kg



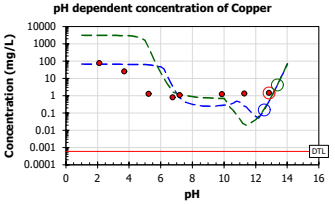
pH dependent concentration of Cobalt



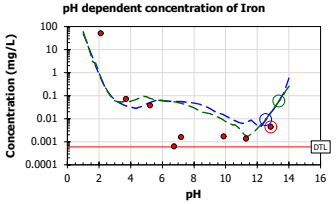
pH dependent concentration of Chromium



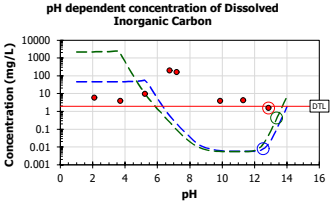
pH dependent concentration of Copper



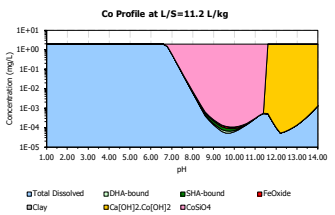
pH dependent concentration of Iron



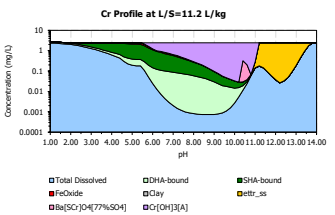
pH dependent concentration of Dissolved Inorganic Carbon



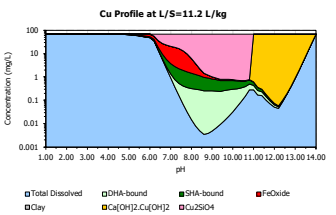
Co Profile at L/S=11.2 L/kg



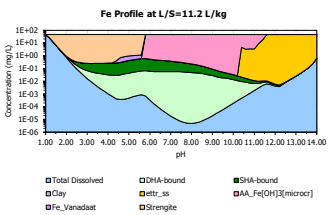
Cr Profile at L/S=11.2 L/kg



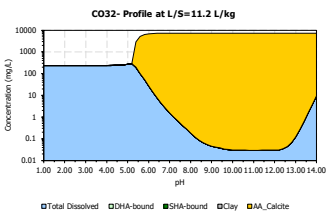
Cu Profile at L/S=11.2 L/kg



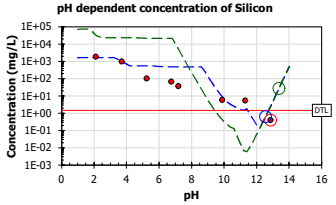
Fe Profile at L/S=11.2 L/kg



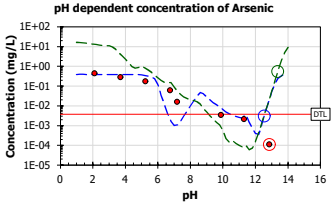
CO32- Profile at L/S=11.2 L/kg



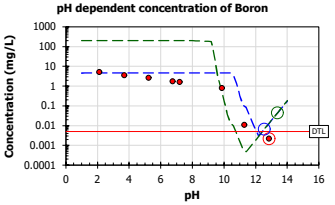
pH dependent concentration of Silicon



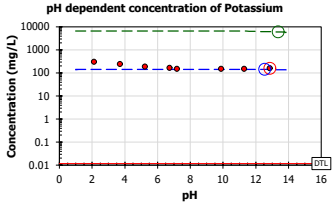
pH dependent concentration of Arsenic



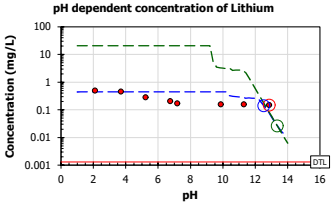
pH dependent concentration of Boron



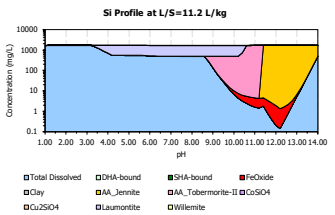
pH dependent concentration of Potassium



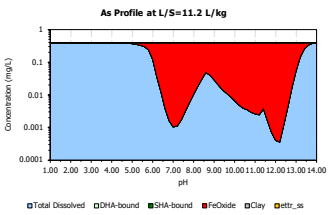
pH dependent concentration of Lithium



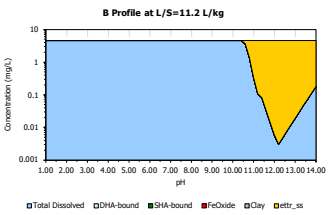
Si Profile at L/S=11.2 L/kg



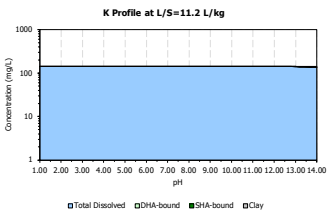
As Profile at L/S=11.2 L/kg



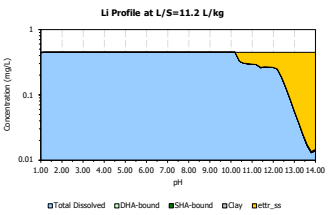
B Profile at L/S=11.2 L/kg



K Profile at L/S=11.2 L/kg



Li Profile at L/S=11.2 L/kg



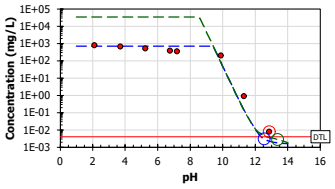
pH dependent concentration of Magnesium

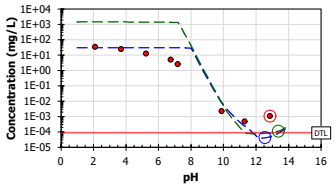
pH dependent concentration of Manganese

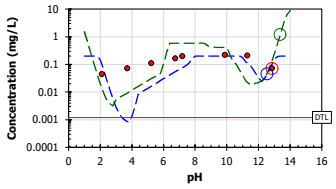
pH dependent concentration of Molybdenum

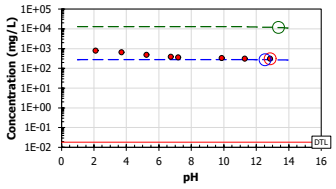
pH dependent concentration of Sodium

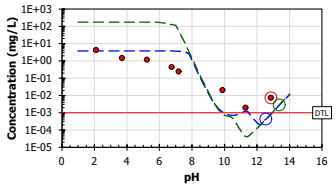
pH dependent concentration of Nickel

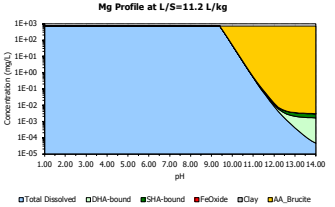

Concentration (mg/L)
pH
DTL

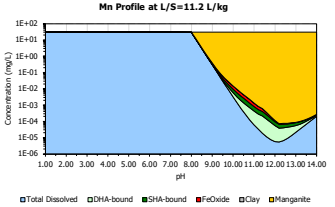

Concentration (mg/L)
pH
DTL

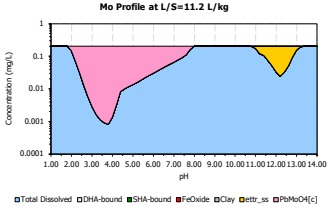

Concentration (mg/L)
pH
DTL

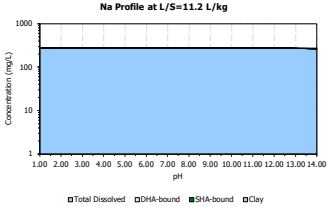

Concentration (mg/L)
pH
DTL

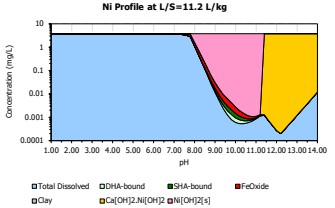

Concentration (mg/L)
pH
DTL

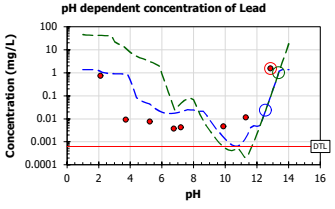

Mg Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
AA_Brucite

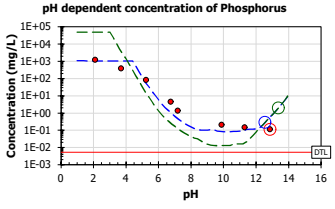

Mn Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Manganite

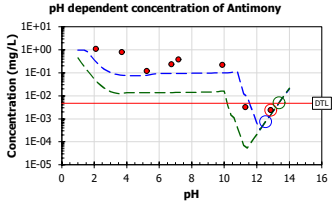

Mo Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss
PbMoO4[c]

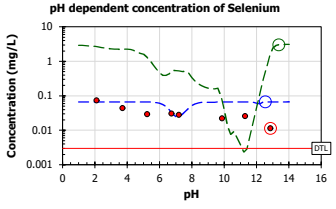

Na Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
Clay

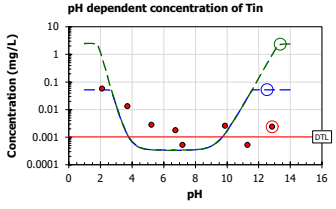

Ni Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Ca[OH]2.Ni[OH]2
Ni[OH]2[s]

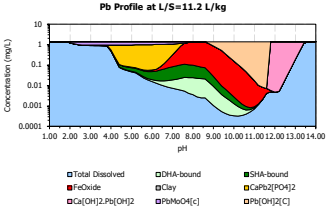

pH dependent concentration of Lead
Concentration (mg/L)
pH
DTL

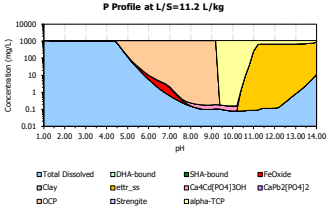

pH dependent concentration of Phosphorus
Concentration (mg/L)
pH
DTL

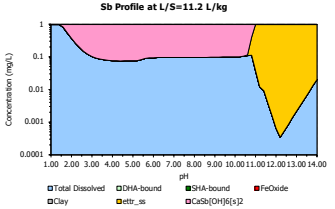

pH dependent concentration of Antimony
Concentration (mg/L)
pH
DTL

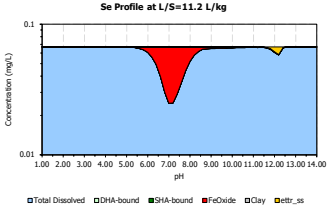

pH dependent concentration of Selenium
Concentration (mg/L)
pH
DTL

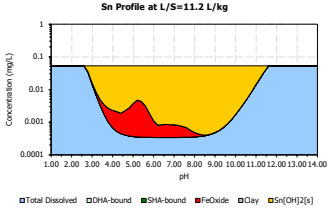

pH dependent concentration of Tin
Concentration (mg/L)
pH
DTL

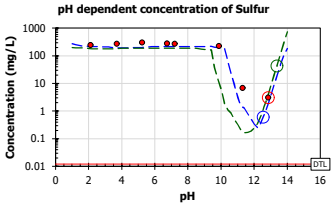

Pb Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
CaPb2[PO4]2
Ca[OH]2.Pb[OH]2
PbMoO4[c]
Pb[OH]2[C]

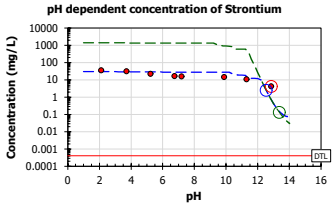

P Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss
Ca4Cd[PO4]3OH
CaPb2[PO4]2
OCP
Strengite
alpha-TCP

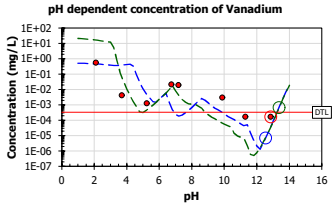

Sb Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss
CaSb[OH]6[s]2

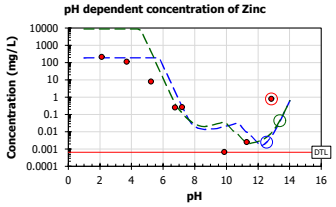

Se Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss

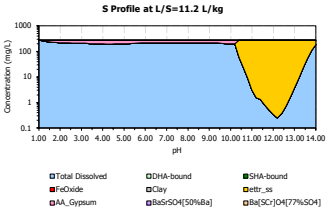

Sn Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Sn[OH]2[s]

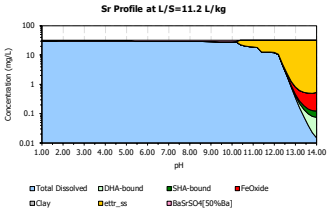

pH dependent concentration of Sulfur
Concentration (mg/L)
pH
DTL

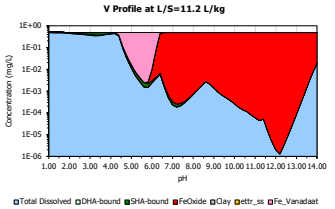

pH dependent concentration of Strontium
Concentration (mg/L)
pH
DTL

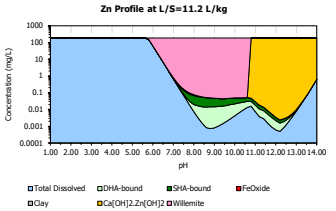

pH dependent concentration of Vanadium
Concentration (mg/L)
pH
DTL


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


S Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss
AA_Gypsum
BaSrSO4[50%Ba]
Ba[SCr]O4[77%SO4]


Sr Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss
BaSrSO4[50%Ba]


V Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ettr_ss
Fe_Vanadaat


Zn Profile at L/S=11.2 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Ca[OH]2.Zn[OH]2
Willemite

Sample MSWI bottom ash alkaline TW

Residual details, concentrations

	Residuals as log(model/sample)						Own pH		
Fraction	*8*	*7*	*6*	*5*	*4*	*3*	*2*	*1*	*Total Avg*
pH	*2.12*	*3.71*	*5.24*	*6.75*	*7.20*	*9.88*	*11.3*	*12.9*	*Deviation*
Al	-0.04	-0.07	-2.34	0.11	-0.09	-2.14	-0.15	0.86	0.41
As	-0.04	0.14	0.30	-1.47	-1.15	0.36	0.16	2.33	0.38
B	-0.04	0.11	0.25	0.43	0.46	0.77	0.95	0.81	0.20
Ba	0.01	0.45	0.57	0.22	0.02	-0.27	0.06	-0.97	0.16
Br	-	-	-	-	-	-	-	-	-
Ca	-0.04	0.02	0.06	-0.01	0.01	0.02	-0.11	-0.53	0.07
Cd	-0.01	-0.04	0.45	1.02	1.33	0.86	0.51	0.83	0.27
Cl	-	-	-	-	-	-	-	-	-
Co	0.54	-0.04	0.51	0.95	0.24	-1.37	0.02	-0.57	0.24
CO32-	-	-	-	-	-	-	-	-	-
Cr	-0.08	0.90	1.67	0.83	0.68	-0.69	-0.30	0.21	0.29
Cu	-0.04	0.43	1.69	0.64	-0.14	-0.63	-0.73	-0.47	0.27
F	-	-	-	-	-	-	-	-	-
Fe	-1.96	-0.28	0.13	1.97	1.54	0.94	0.73	0.62	0.43
Hg	-	-	-	-	-	-	-	-	-
K	-0.32	-0.23	-0.12	-0.06	-0.03	-0.02	-0.01	-0.04	0.05
Li	-0.04	0.00	0.21	0.35	0.43	0.46	0.25	-0.29	0.11
Mg	-0.04	0.04	0.15	0.28	0.31	-0.38	-0.78	-0.55	0.14
Mn	-0.04	0.11	0.39	0.79	1.07	0.60	-0.29	-1.33	0.25
Mo	0.31	-1.92	-0.82	-0.47	-0.40	-0.03	-0.26	0.18	0.28
Na	-0.44	-0.37	-0.23	-0.14	-0.11	-0.07	-0.04	-0.04	0.08
Ni	-0.04	0.41	0.51	0.92	1.18	-1.26	-0.21	-0.91	0.28
NO3	-	-	-	-	-	-	-	-	-
P	-0.05	0.45	-0.19	-0.64	-0.46	-0.39	-0.15	0.73	0.16
Pb	0.19	1.99	0.75	0.68	0.69	-0.45	-0.85	-1.19	0.35
S	-0.05	-0.13	-0.17	-0.10	-0.10	-0.04	-0.68	-0.18	0.09
Sb	-0.55	-0.99	-0.18	-0.38	-0.60	-0.34	0.53	-0.18	0.19
Se	-0.04	0.19	0.36	0.03	-0.04	0.48	0.41	0.77	0.14
Si	-0.04	0.01	0.73	0.87	1.13	0.20	-0.52	0.84	0.24
Sn	-0.04	-1.03	-0.90	-0.72	-0.18	-0.26	1.73	1.35	0.34
Sr	-0.06	-0.01	0.14	0.24	0.27	0.31	0.15	-0.79	0.12
Th	-	-	-	-	-	-	-	-	-
U	-	-	-	-	-	-	-	-	-
V	-0.06	1.98	0.57	-1.51	-1.99	-0.95	-0.53	-0.62	0.43
Zn	-0.04	0.23	1.38	0.93	0.03	1.50	0.59	-2.15	0.40
Avg Deviation	0.08	0.15	0.16	0.15	0.15	0.15	0.11	0.18	0.24

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 Deviatio 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.

Values below 1 are considered adequate description