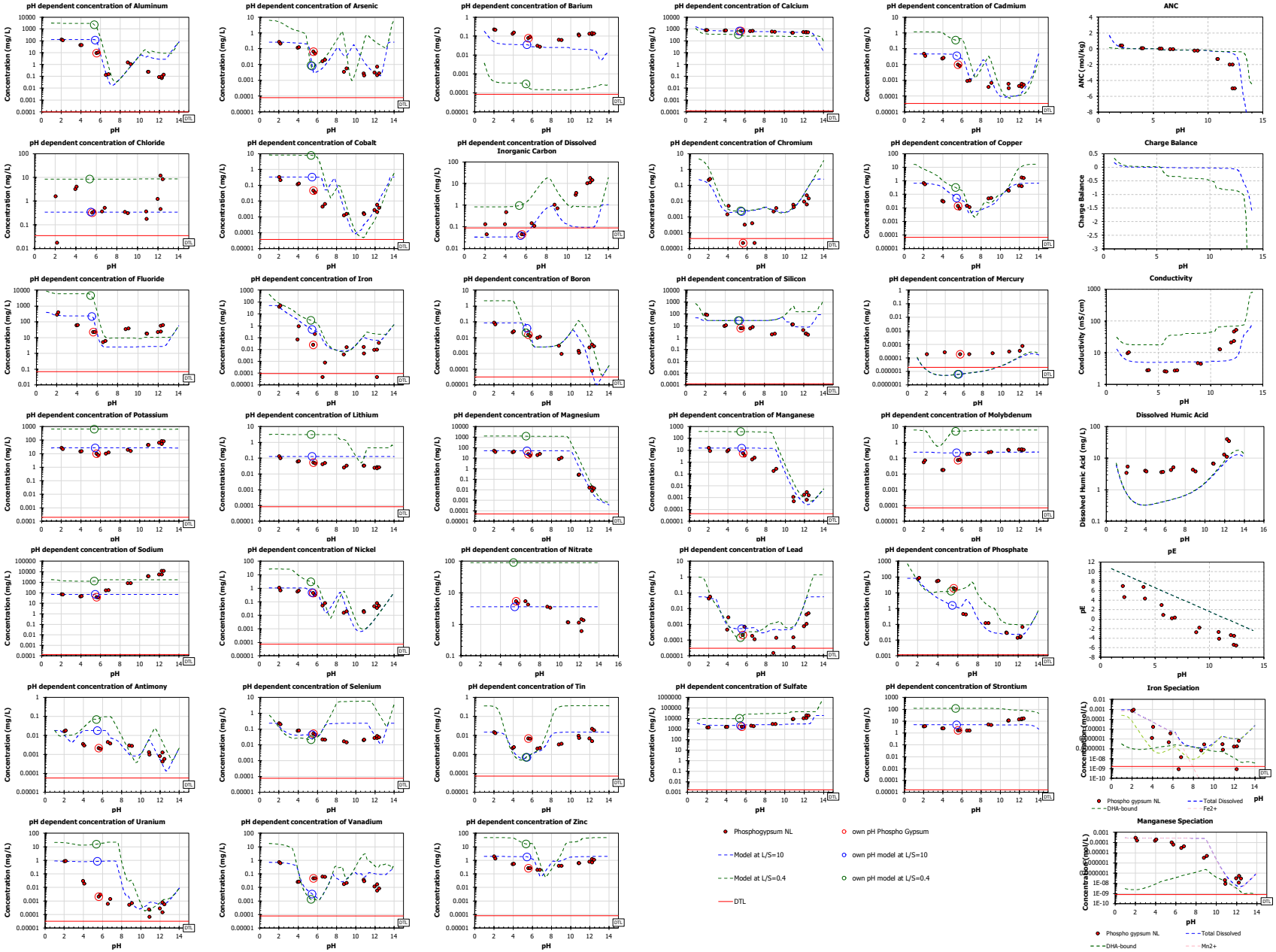
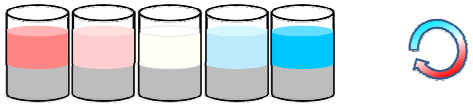
PHOSPHO GYPSUM NL

COMPARISON pH DEPENDENCE WITH MODEL



Object pH Dependent Leaching Test Model
Name Phospho-Gypsum NL

pH Dependent Leaching Test Scenario



Lab Test

Extra L/S Simulation

Lab Test

Model Parameters

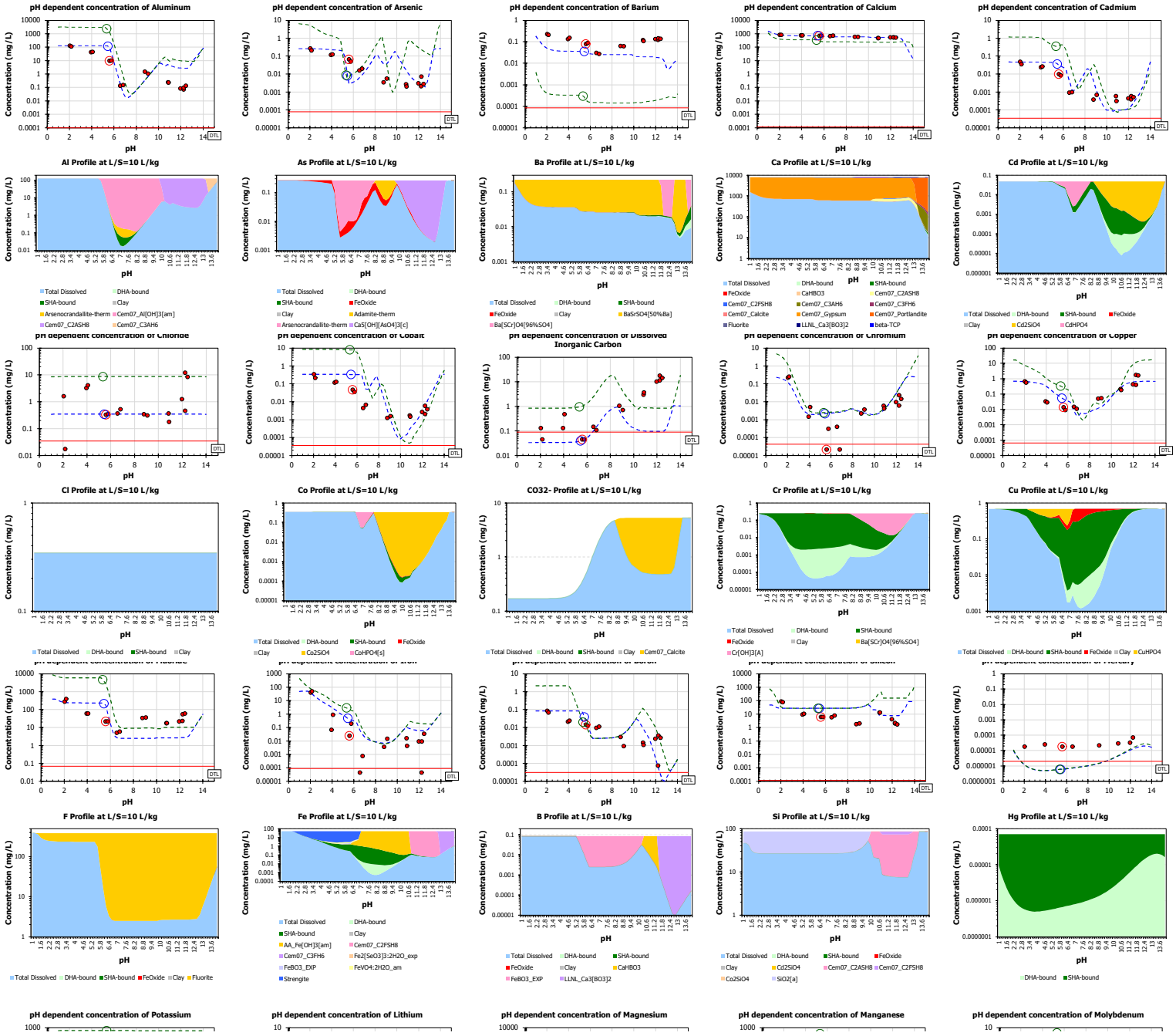
Entity	Unit	Default
c0		-3.717
c1		-2.441
c2		0.7288
c3		-0.1029
c4		0.007015
c5		-0.0001810
Clay	mg/kg	3000
Hydrous Ferric Oxid	mg/kg	200.0
L/S	L/kg	10.000
pE		5.740
pH		5.860
Solid Humic Acid	mg/kg	450.0
Simulated Low L/S	L/kg	0.4000

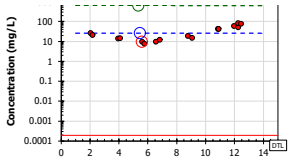
Available Content

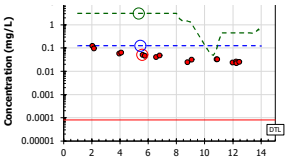
Entity	mg/kg	Entity	mg/kg	Entity	mg/kg
Al	1289	Si	857.3	Sb	0.1800
As	2.630	Hg	0.0007000	Se	2.300
Ba	2.240	K	259.8	Sn	0.1455
Ca	7.845E+04	Li	1.262	SO4	1.885E+05
Cd	0.4760	Mg	494.3	Sr	50.39
Cl	3.445	Mn	152.0	U	8.789
Co	3.390	Mo	2.390	V	7.139
CO32-	52.75	Na	690.7	Zn	19.00
Cr	2.520	Ni	10.50		
Cu	6.810	NO3	35.87		
F	3875	Pb	0.5460		
Fe	495.4	PO4	846.8		
B	0.8489				

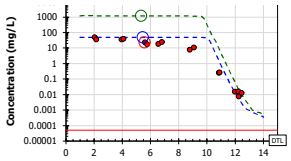
Minerals

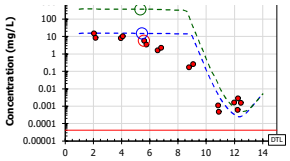
Name	Log(K)	Reaction
AA_Fe[OH]3[am]	16.60	AA_Fe[OH]3[am] + 1 H2O -> 1 Fe[OH]4- + 1 H+
Adamite-therm	12.64	Adamite-therm + 1 H+ -> 1 AsO4-3 + 1 H2O + 2 Zn+2
AlOHSO4	26.23	AlOHSO4 + 3 H2O -> 1 Al[OH]4- + 3 H+ + 1 SO4-2
Antimocrandallite-e	63.00	Antimocrandallite-exp + 8 H2O -> 3 Al[OH]4- + 1 Ca+2 + 3 H+ + 2 Sb[OH]6-
Arsenocrandallite-tl	95.56	Arsenocrandallite-therm + 6 H2O -> 3 Al[OH]4- + 2 AsO4-3 + 1 Ca+2 + 7 H+
B_UO2[OH]2	-8.329	B_UO2[OH]2 + 2 H+ + 1 e- -> 2 H2O + 1 UO2+
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-
Ca3[OH]2[SeO4]2[c	6.477	Ca3[OH]2[SeO4]2[ccc] + 2 H+ -> 3 Ca+2 + 2 H2O + 2 SeO4-2
Ca5[OH][AsO4]3[c]	26.13	Ca5[OH][AsO4]3[c] + 1 H+ -> 3 AsO4-3 + 5 Ca+2 + 1 H2O
CaCO3_Li2CO3	21.30	CaCO3_Li2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 Li+
CaHBO3	-2.097	CaHBO3 + 1 H+ -> 1 Ca+2 + 1 H2BO3-
Carnotite	-3.015	Carnotite + 4 H+ + 1 e- -> 2 H2O + 1 K+ + 1 UO2+ + 1 VO2+
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_C2ASH8	17.40	Cem07_C2ASH8 -> 2 Al[OH]4- + 2 Ca+2 + 3 H2O + 1 H2SiO4-2
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_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
Cem07_Portlandite	-22.79	Cem07_Portlandite + 2 H+ -> 1 Ca+2 + 2 H2O
Co2SiO4	5.289	Co2SiO4 + 2 H+ -> 2 Co+2 + 1 H2SiO4-2
CoHPO4[s]	24.48	CoHPO4[s] -> 1 Co+2 + 1 H+ + 1 PO4-3
Cr[OH]3[A]	68.13	Cr[OH]3[A] + 1 H2O -> 1 CrO4-2 + 5 H+ + 3 e-
Cryolite	56.84	Cryolite + 4 H2O -> 1 Al[OH]4- + 6 F- + 4 H+ + 3 Na+
CuHPO4	26.00	CuHPO4 -> 1 Cu+2 + 1 H+ + 1 PO4-3
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-
FeBO3_EXP	32.48	FeBO3_EXP + 2 H2O -> 1 Fe[OH]4- + 2 H+ + 1 H2BO3-
FeVO4:2H2O_am	23.48	FeVO4:2H2O_am + 2 H2O -> 1 Fe[OH]4- + 1 VO2+
Fluorite	10.50	Fluorite -> 1 Ca+2 + 2 F-
Li2_CaO_Al2O3_SiO2_8H2O[s]	22.69	Li2_CaO_Al2O3_SiO2_8H2O[s] -> 2 Al[OH]4- + 1 Ca+2 + 3 H2O + 1 H2SiO4-2 + 2 Li+
LLNL_Ca3[BO3]2	-24.52	LLNL_Ca3[BO3]2 + 4 H+ -> 3 Ca+2 + 2 H2BO3-
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
NiHPO4	25.00	NiHPO4 -> 1 H+ + 1 Ni+2 + 1 PO4-3
PATCH_Fe2[MoO4]3[1]	82.02	PATCH_Fe2[MoO4]3[1] + 8 H2O -> 2 Fe[OH]4- + 8 H+ + 3 MoO4-2
Pb[OH]2[C]	-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
Pb[Sb[OH]6]2_exp	29.00	Pb[Sb[OH]6]2_exp -> 1 Pb+2 + 2 Sb[OH]6-
PbMoO4[c]	15.80	PbMoO4[c] -> 1 MoO4-2 + 1 Pb+2
PbOH[Sb[OH]6]_exp3	13.00	PbOH[Sb[OH]6]_exp3 + 1 H+ -> 1 H2O + 1 Pb+2 + 1 Sb[OH]6-
SiO2[a]	24.64	SiO2[a] + 2 H2O -> 2 H+ + 1 H2SiO4-2
Spodumene2	58.00	Spodumene2 + 6 H2O -> 1 Al[OH]4- + 4 H+ + 2 H2SiO4-2 + 1 Li+
Strengite	48.00	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
Tyuyamunite	-4.825	Tyuyamunite + 4 H+ + 1 e- -> 0.5 Ca+2 + 2 H2O + 1 UO2+ + 1 VO2+
ZnHPO4	24.48	ZnHPO4 -> 1 H+ + 1 PO4-3 + 1 Zn+2

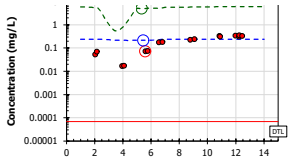

pH dependent concentration of Aluminum
pH dependent concentration of Arsenic
pH dependent concentration of Barium
pH dependent concentration of Calcium
pH dependent concentration of Cadmium
Al Profile at L/S=10 L/kg
As Profile at L/S=10 L/kg
Ba Profile at L/S=10 L/kg
Ca Profile at L/S=10 L/kg
Cd Profile at L/S=10 L/kg
pH dependent concentration of Chloride
pH dependent concentration of Cobalt
pH dependent concentration of Dissolved Inorganic Carbon
pH dependent concentration of Chromium
pH dependent concentration of Copper
Cl 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
F 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
Hg Profile at L/S=10 L/kg
pH dependent concentration of Potassium
pH dependent concentration of Lithium
pH dependent concentration of Magnesium
pH dependent concentration of Manganese
pH dependent concentration of Molybdenum
Concentration (mg/L)
pH
DTL
Total Dissolved
DHA-bound
SHA-bound
Clay
FeOxide
Arsenocrandallite-therm
Cem07_Al[OH]3[am]
Cem07_C2ASH8
Cem07_C3AH6
Adamite-therm
Ca5[OH][AsO4]3[c]
BaSrSO4[50%Ba]
Ba[SCr]O4[96%SO4]
CaHBO3
Cem07_C2ASH8
Cem07_C2FSH8
Cem07_C3AH6
Cem07_C3FH6
Cem07_Calcite
Cem07_Gypsum
Cem07_Portlandite
Fluorite
LLNL_Ca3[BO3]2
beta-TCP
Cd2SiO4
CdHPO4
Co2SiO4
CoHPO4[s]
Cem07_Calcite
Ba[SCr]O4[96%SO4]
Cr[OH]3[A]
CuHPO4
AA_Fe[OH]3[am]
Fe2[SeO3]3:2H2O_exp
FeBO3_EXP
FeVO4:2H2O_am
Strengite
FeBO3_EXP
Cem07_C2FSH8
Cem07_C3FH6
Clay
Cd2SiO4
Co2SiO4
SiO2[a]



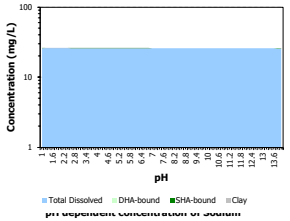




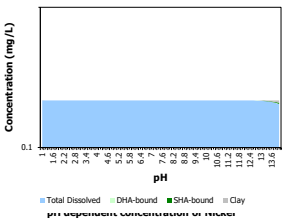




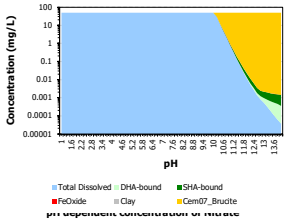
K Profile at L/S=10 L/kg



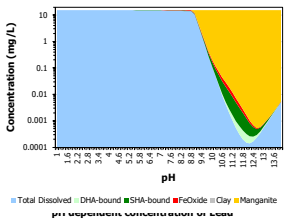
Li Profile at L/S=10 L/kg



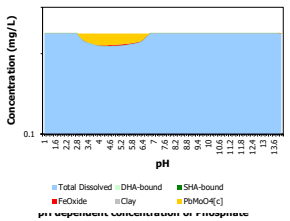
Mg Profile at L/S=10 L/kg

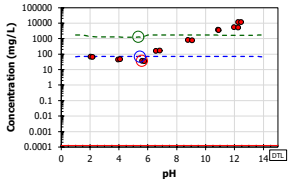


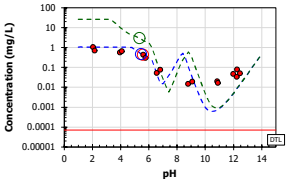
Mn Profile at L/S=10 L/kg

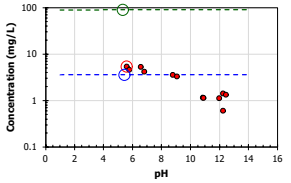


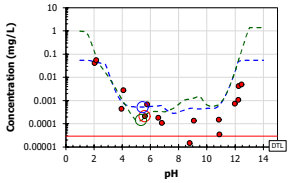
Mo Profile at L/S=10 L/kg

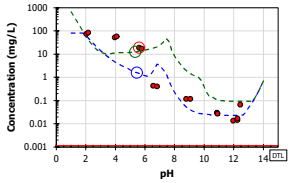




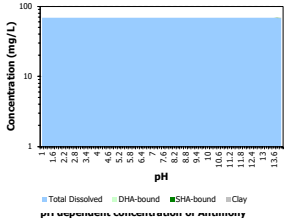




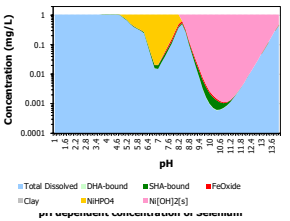




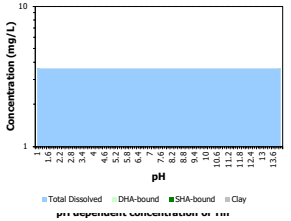
Na Profile at L/S=10 L/kg



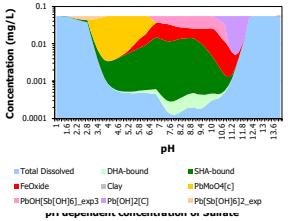
Ni Profile at L/S=10 L/kg



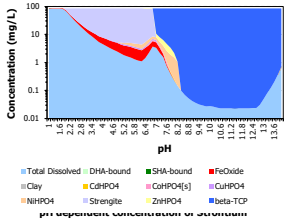
NO3 Profile at L/S=10 L/kg

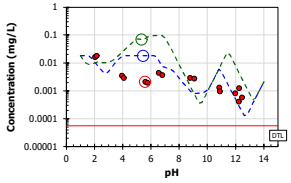


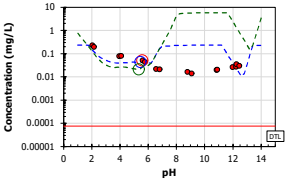
Pb Profile at L/S=10 L/kg

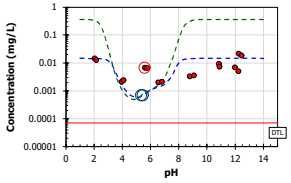


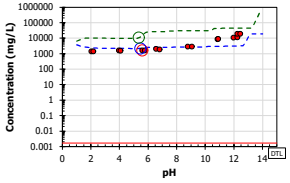
PO4 Profile at L/S=10 L/kg

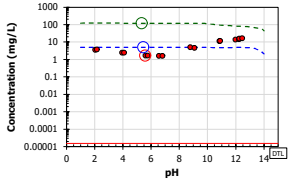




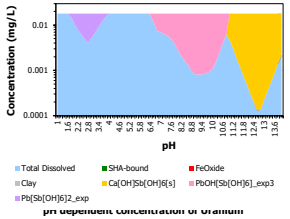




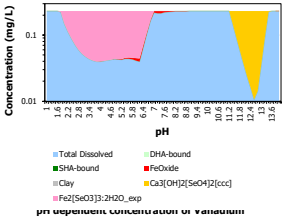




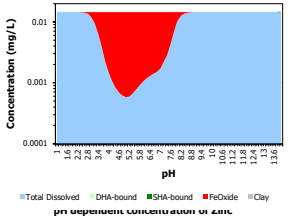
Sb Profile at L/S=10 L/kg



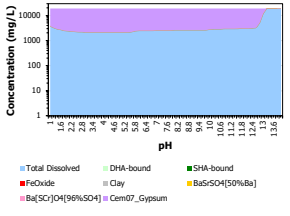
Se Profile at L/S=10 L/kg



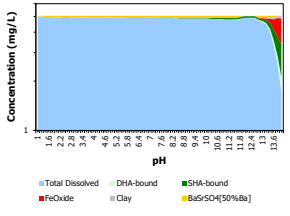
Sn Profile at L/S=10 L/kg

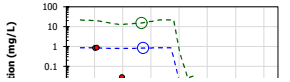


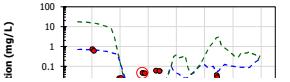
SO4 Profile at L/S=10 L/kg

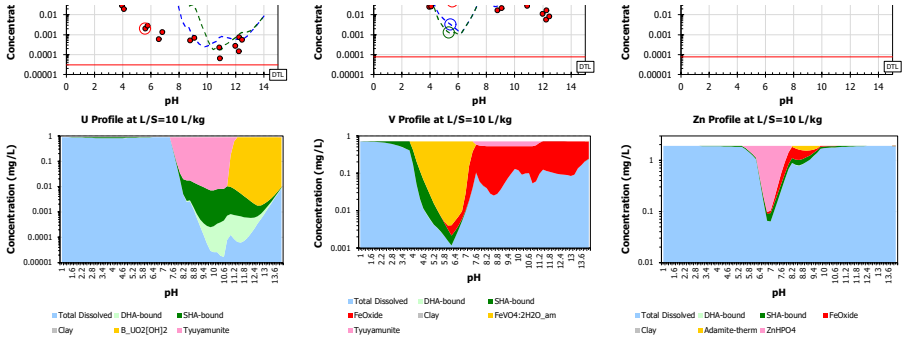


Sr Profile at L/S=10 L/kg








Concentrat
pH
DTL
U Profile at L/S=10 L/kg
Concentration (mg/L)
Total Dissolved
DHA-bound
SHA-bound
Clay
B_UO2[OH]2
Tyuyamunite
V Profile at L/S=10 L/kg
FeOxide
FeVO4:2H2O_am
Zn Profile at L/S=10 L/kg
ZnHPO4
Adamite-therm

Model Comparison: residuals - Concentration

Name **Phospho-Gypsum 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 Devi 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*	*16*	*7*	*15*	*6*	*14*	*5*	*13*	*12*	*4*	*3*	*11*	*2*	*10*	*1*	*9*	*Total Avg*
pH	*2.04*	*2.16*	*3.95*	*4.08*	*5.60*	*5.77*	*6.56*	*6.81*	*8.78*	*9.07*	*10.9*	*10.9*	*12.0*	*12.2*	*12.3*	*12.4*	*Deviation*
Al	0.00	0.06	0.48	0.46	1.01	0.52	0.09	-0.60	-0.60	-0.18	1.30	1.30	1.52	1.58	1.46	1.31	0.24
As	0.00	0.10	0.30	0.26	-1.35	-1.21	-0.41	-0.34	1.03	0.84	0.77	0.85	0.00	0.07	-0.47	-0.11	0.17
Ba	-0.65	-0.66	-0.56	-0.62	-0.37	-0.47	-0.05	0.00	-0.40	-0.38	-0.78	-0.74	-0.84	-0.82	-0.89	-0.88	0.16
Ca	0.01	0.00	-0.02	-0.02	0.00	-0.04	-0.03	-0.06	0.01	0.02	0.05	0.05	0.02	0.03	0.04	0.07	0.01
Cd	0.00	0.13	0.29	0.24	0.51	0.53	0.63	0.11	1.01	0.23	-0.76	-0.48	-0.55	-0.36	-0.53	-0.31	0.12
Cl	-0.67	1.29	-0.97	-1.07	0.02	-0.01	-0.03	-0.18	0.00	0.05	-0.03	0.29	-0.56	-0.13	-1.54	-1.39	0.19
Co	0.00	0.20	0.46	0.42	0.85	0.97	1.54	0.90	0.45	-0.19	-0.72	-0.64	0.01	0.45	0.00	0.46	0.16
CO32-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Cr	-0.27	-0.41	0.17	-0.39	2.01	0.86	0.80	2.09	0.10	-0.18	-0.22	-0.04	0.49	0.94	0.38	0.77	0.22
Cu	-0.02	0.06	1.02	1.01	0.53	0.66	-0.28	-0.48	-0.60	-0.53	0.11	0.20	0.16	0.22	-0.44	-0.39	0.13
F	-0.04	-0.19	0.60	0.59	0.91	0.46	-0.26	-0.37	-1.13	-1.17	-0.82	-0.81	-0.91	-0.93	-1.31	-1.34	0.21
Fe	-0.02	-0.21	1.69	0.49	1.24	0.27	3.16	1.60	0.28	-0.31	0.82	1.37	0.82	3.11	0.79	0.23	0.35
B	0.00	0.10	0.61	0.55	0.21	0.00	-0.58	-0.64	0.08	0.71	0.80	0.87	-1.06	-0.10	-1.80	-2.06	0.22
Si	-0.50	-0.45	0.46	0.42	0.66	0.65	0.67	0.54	1.22	1.20	-0.17	-0.18	0.27	0.58	0.54	0.66	0.16
Hg	-1.18	-	-1.70	-	-1.46	-	-1.38	-	-	-1.16	-0.81	-	-0.48	-	-0.75	-	0.42
K	0.00	0.09	0.27	0.25	0.43	0.53	0.42	0.34	0.15	0.23	-0.22	-0.21	-0.37	-0.29	-0.50	-0.47	0.08
Li	0.00	0.11	0.34	0.30	0.40	0.44	0.49	0.42	0.71	0.59	0.59	0.58	0.73	0.68	0.76	0.70	0.13
Mg	0.00	0.13	0.15	0.10	0.32	0.44	0.42	0.30	0.80	0.65	0.76	0.66	-0.05	-0.47	-0.16	-0.66	0.11
Mn	0.00	0.26	0.27	0.17	0.43	0.65	0.97	0.82	1.92	1.48	0.60	0.90	-0.69	-0.37	-1.04	-0.77	0.21
Mo	0.66	0.54	1.10	1.09	0.48	0.47	0.11	0.12	0.02	0.00	-0.15	-0.11	-0.16	-0.11	-0.18	-0.14	0.12
Na	0.00	0.02	0.19	0.17	0.27	0.29	-0.36	-0.40	-1.06	-1.05	-1.72	-1.72	-1.89	-1.88	-2.23	-2.23	0.32
Ni	0.00	0.18	0.27	0.20	-0.03	0.07	-0.04	-0.69	0.90	0.23	-1.41	-1.33	-0.98	-0.59	-0.94	-0.56	0.17
NO3	-	-	-	-	-0.18	-0.10	-0.17	-0.06	0.00	0.03	0.49	0.50	0.51	0.77	0.40	0.43	0.11
Pb	0.04	-0.09	0.32	-0.55	0.40	-0.10	0.51	0.74	1.49	0.54	0.61	1.28	1.38	1.65	1.07	1.05	0.22
PO4	-0.09	-0.24	-1.05	-1.13	-1.11	-1.11	0.66	0.95	-0.33	-0.46	-0.11	-0.07	0.23	0.21	0.14	-0.45	0.16
Sb	-0.20	-0.33	0.69	0.79	0.94	0.97	0.44	0.30	-0.45	-0.53	0.64	0.75	-0.19	-0.16	-0.64	-0.50	0.15
Se	-0.21	-0.22	-0.29	-0.30	-0.07	-0.01	0.63	0.89	1.15	1.21	1.07	1.05	0.18	-0.08	-0.20	-0.32	0.16
Sn	0.00	0.05	-0.10	-0.26	-0.95	-0.87	-0.16	-0.14	0.64	0.61	0.20	0.30	0.33	0.47	-0.17	-0.10	0.11
SO4	0.24	0.22	0.14	0.14	0.14	0.18	0.10	0.13	-0.04	-0.04	-0.46	-0.47	-0.54	-0.56	-0.79	-0.77	0.10
Sr	0.14	0.13	0.31	0.30	0.46	0.47	0.49	0.49	-0.02	0.02	-0.36	-0.38	-0.45	-0.47	-0.51	-0.52	0.10
U	0.00	-0.02	1.44	1.62	2.62	2.47	3.16	2.81	0.52	0.01	0.51	1.06	0.34	0.61	-0.11	0.05	0.38
V	-0.02	0.04	0.92	0.61	-1.23	-1.32	-1.33	-1.03	0.22	0.29	0.18	0.31	0.96	1.23	0.76	1.05	0.21
Zn	0.00	0.15	0.56	0.54	0.81	0.76	0.01	-0.46	0.33	0.40	0.47	0.48	0.39	0.45	0.20	0.25	0.11
Avg Deviati	0.06	0.06	0.13	0.11	0.16	0.14	0.18	0.15	0.13	0.11	0.13	0.14	0.13	0.17	0.15	0.15	0.18

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