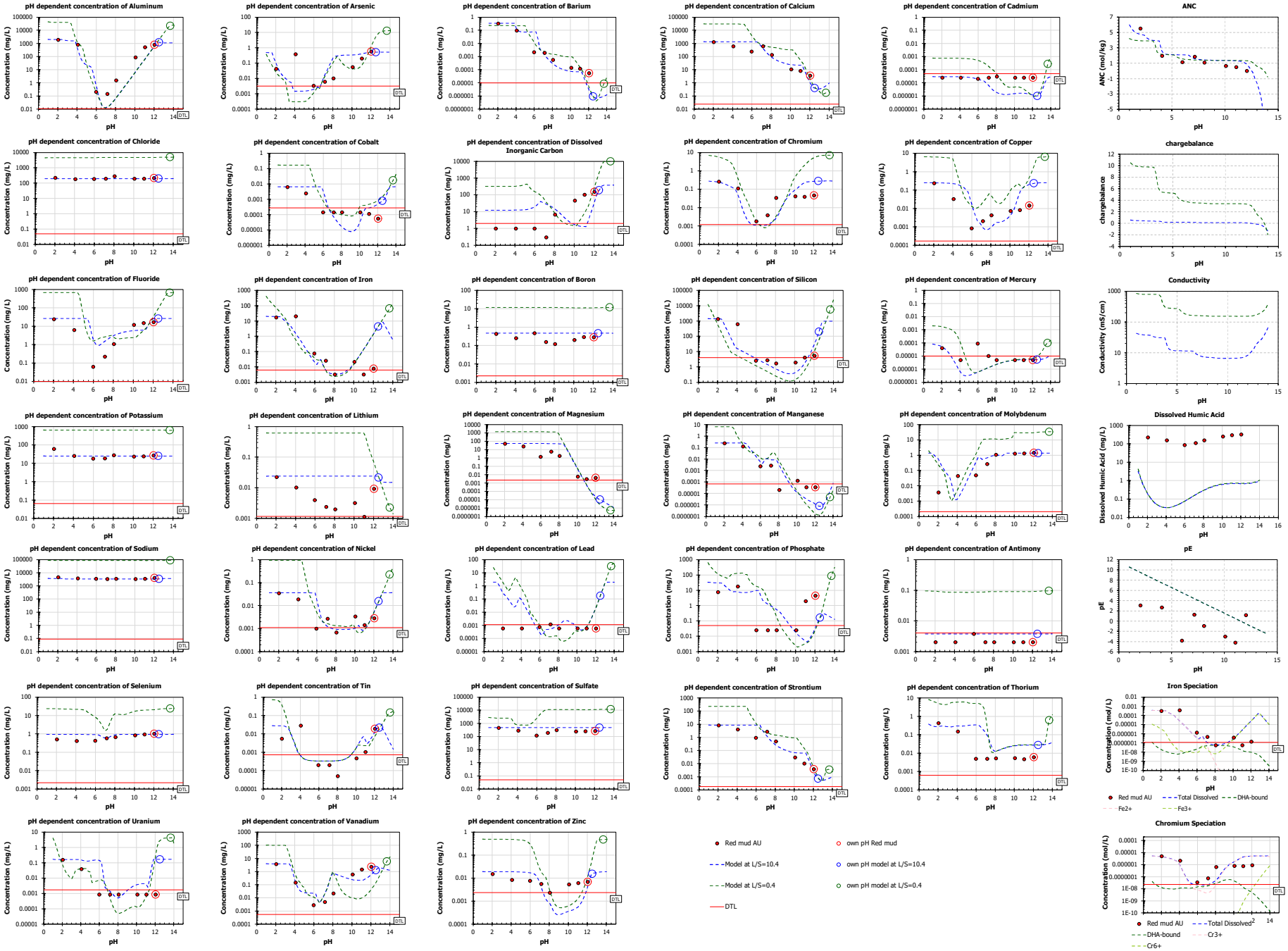
RED MUD AU

COMPARISON pH DEPENDENCE WITH MODEL



Object pH Dependent Leaching Test Model
Name Red Mud

pH Dependent Leaching Test Scenario

Lab Test

Extra L/S Simulation

Lab Test

Model Parameters

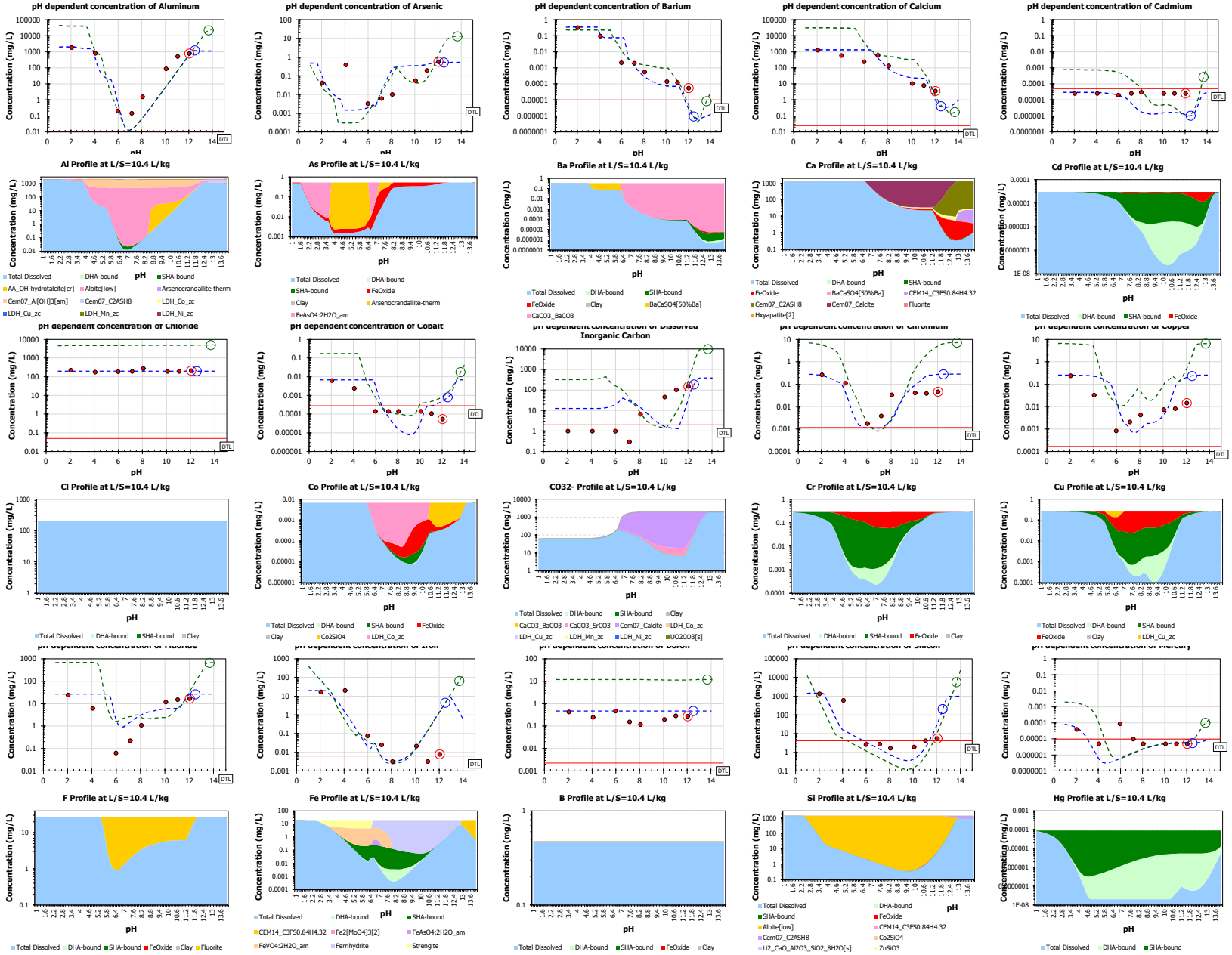
Entity	Unit	Default	Available Content Entity	mg/kg	Entity	mg/kg	Entity	mg/kg
c0		-3.777	Al	2.103E+04	B	4.877	Sb	0.03929
c1		-2.507	As	5.459	Si	1.504E+04	Se	9.886
c2		0.5249	Ba	3.609	Hg	0.0009279	Sn	0.2910
c3		-0.04144	Br	35.00	K	259.9	SO4	4940
c4		0.001130	Ca	1.415E+04	Li	0.2493	Sr	92.09
c5		0	Cd	0.0003107	Mg	568.0	Th	4.780
Clay	mg/kg	1.000E+04	Cl	2046	Mn	2.596	U	1.771
Hydrous Ferric Oxide	mg/kg	1200	Co	0.06989	Mo	14.07	V	41.69
L/S	L/kg	10.35	CO32-	1.994E+04	Na	3.904E+04	Zn	0.2000
pE		-0.5000	Cr	2.919	Ni	0.3826		
pH		12.04	Cu	2.649	NO3	0.7000		
Solid Humic Acid	mg/kg	120.0	F	274.9	Pb	20.01		
Simulated Low L/S	L/kg	0.4000	Fe	208.6	PO4	550.0		

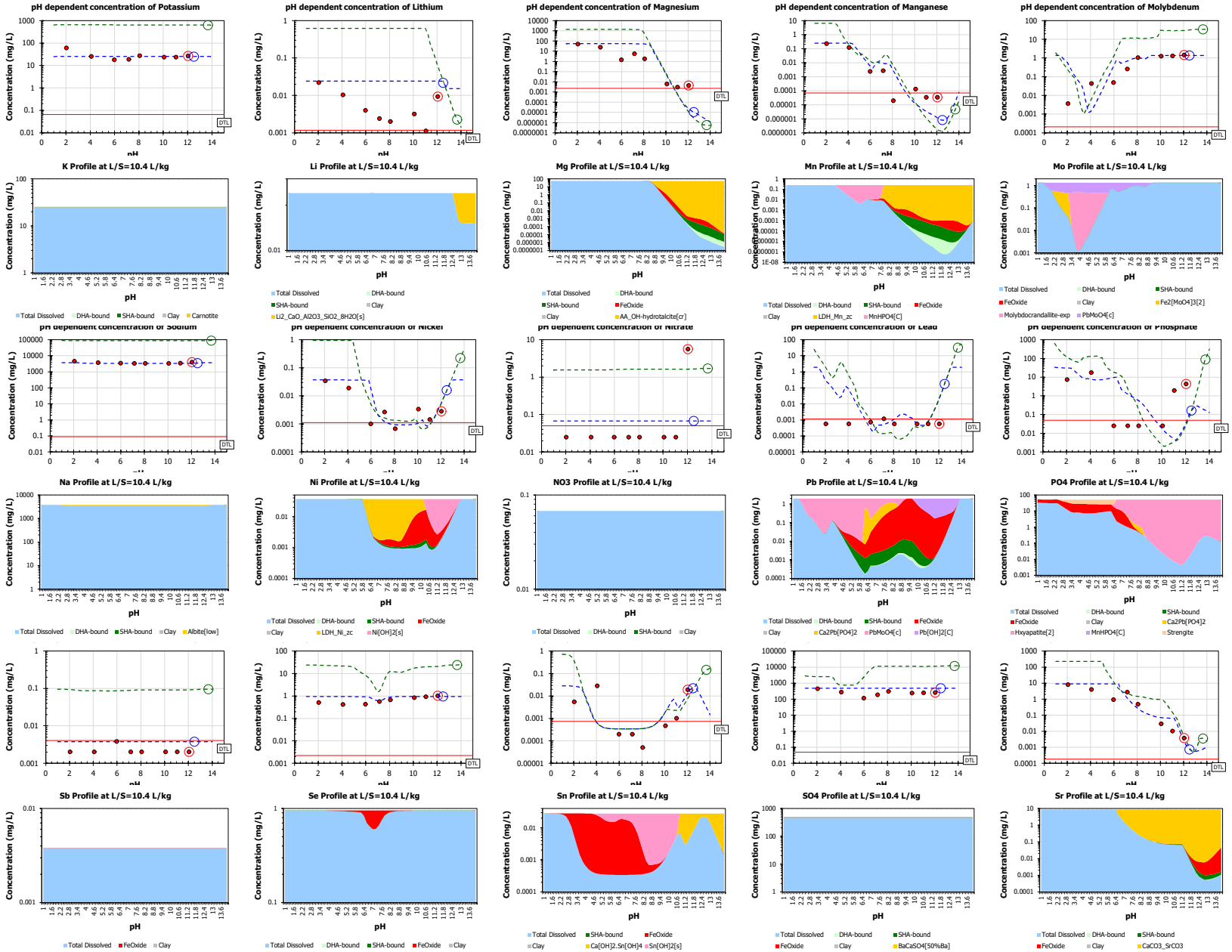
Solid Solutions

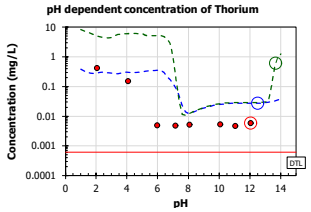
End Member	Log(K)	Reaction	End Member	Log(K)	Reaction
AsO4_Ettringite_ss	26.79	AsO4_Ettringite_ss + 1 H+ + 8 H2O -> 2 Al[OH]4- + 3 AsO4-3 + 6 Ca+2 + 1 ettr_ss	MoO4_Ettringite_ss	-9.592	MoO4_Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 MoO4-2 + 1 ettr_ss
Ba_Ettringite_ss	4.008	Ba_Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ba+2 + 3 SO4-2 + 1 ettr_ss	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
BO3_Ettringite_ss	-46.87	BO3_Ettringite_ss + 7 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 H2BO3- + 1 ettr_ss	Sb[OH]6-_Ettringite_ss	-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
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	SeO4-2_Ettringite_ss	4.408	SeO4-2_Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 SeO4-2 + 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	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

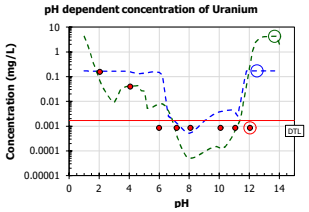
Minerals

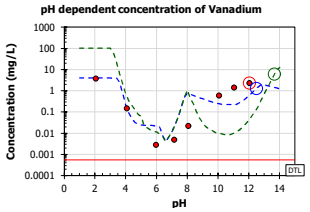
Name	Log(K)	Reaction	Name	Log(K)	Reaction
AA_OH-hydrotalcite[cr]	-27.97	AA_OH-hydrotalcite[cr] + 6 H+ -> 2 Al[OH]4- + 9 H2O + 4 Mg+2	Ferrihydrite	16.71	Ferrihydrite + 1 H2O -> 1 Fe[OH]4- + 1 H+
Albite[low]	85.27	Albite[low] + 8 H2O -> 1 Al[OH]4- + 6 H+ + 3 H2SiO4-2 + 1 Na+	FeVO4:2H2O_am	23.48	FeVO4:2H2O_am + 2 H2O -> 1 Fe[OH]4- + 1 VO2+
Arsenocrandallite-therm	95.56	Arsenocrandallite-therm + 6 H2O -> 3 Al[OH]4- + 2 AsO4-3 + 1 Ca+2 + 7 H+	Fluorite	10.96	Fluorite -> 1 Ca+2 + 2 F-
BaCaSO4[50%Ba]	7.412	BaCaSO4[50%Ba] -> 0.5 Ba+2 + 0.5 Ca+2 + 1 SO4-2	Hxyapatite[2]	38.15	Hxyapatite[2] + 1 H+ -> 5 Ca+2 + 1 H2O + 3 PO4-3
beta-TCP	28.93	beta-TCP -> 3 Ca+2 + 2 PO4-3	LDH_Co_zc	60.01	LDH_Co_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 3 Co+2 + 1 H+
Ca[OH]2.Cu[OH]2	-28.52	Ca[OH]2.Cu[OH]2 + 4 H+ -> 1 Ca+2 + 1 Cu+2 + 4 H2O	LDH_Cu_zc	58.21	LDH_Cu_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 3 Cu+2 + 1 H+
Ca[OH]2.Sn[OH]4	-39.40	Ca[OH]2.Sn[OH]4 + 6 H+ + 2 e- -> 1 Ca+2 + 6 H2O + 1 Sn+2	LDH_Mn_zc	10.21	LDH_Mn_zc + 3 H+ -> 1 Al[OH]4- + 1 CO3-2 + 3 H2O + 3 Mn+2
Ca2Pb[PO4]2	36.87	Ca2Pb[PO4]2 -> 2 Ca+2 + 2 PO4-3 + 1 Pb+2	LDH_Ni_zc	57.91	LDH_Ni_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 1 H+ + 3 Ni+2
CaCO3_BaCO3	23.00	CaCO3_BaCO3 -> 1 Ba+2 + 2 CO3-2 + 1 Ca+2	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+
CaCO3_SrCO3	19.85	CaCO3_SrCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Sr+2	MnHPO4[C]	25.40	MnHPO4[C] -> 1 H+ + 1 Mn+2 + 1 PO4-3
Carnotite	-3.015	Carnotite + 4 H+ + 1 e- -> 2 H2O + 1 K+ + 1 UO2+ + 1 VO2+	Molybdocrandallite-exp	86.00	Molybdocrandallite-exp + 6 H2O -> 3 Al[OH]4- + 1 Ca+2 + 7 H+ + 3 MoO4-2
Cem07_Al[OH]3[am]	13.76	Cem07_Al[OH]3[am] + 1 H2O -> 1 Al[OH]4- + 1 H+	Ni[OH]2[s]	-10.80	Ni[OH]2[s] + 2 H+ -> 2 H2O + 1 Ni+2
Cem07_C2ASH8	17.40	Cem07_C2ASH8 -> 2 Al[OH]4- + 2 Ca+2 + 3 H2O + 1 H2SiO4-2	Pb[OH]2[C]	-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
Cem07_Calcite	8.485	Cem07_Calcite -> 1 CO3-2 + 1 Ca+2	PbMoO4[c]	15.80	PbMoO4[c] -> 1 MoO4-2 + 1 Pb+2
Cem07_Gypsum	4.583	Cem07_Gypsum -> 1 Ca+2 + 2 H2O + 1 SO4-2	Schoepite	-8.189	Schoepite + 2 H+ + 1 e- -> 3 H2O + 1 UO2+
CEM14_C3FS0.84H4.32	-1.915	CEM14_C3FS0.84H4.32 + 2.32 H+ -> 3 Ca+2 + 2 Fe[OH]4- + 5.68 H2O + 0.84 H2SiO4-2	Sn[OH]2[s]	1.447	Sn[OH]2[s] + 2 H+ -> 2 H2O + 1 Sn+2
Co2SiO4	6.289	Co2SiO4 + 2 H+ -> 2 Co+2 + 1 H2SiO4-2	Strengite	48.00	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
Fe2[MoO4]3[2]	86.35	Fe2[MoO4]3[2] + 8 H2O -> 2 Fe[OH]4- + 8 H+ + 3 MoO4-2	UO2CO3[s]	18.67	UO2CO3[s] + 1 e- -> 1 CO3-2 + 1 UO2+
FeAsO4:2H2O_am	49.70	FeAsO4:2H2O_am + 2 H2O -> 1 AsO4-3 + 1 Fe[OH]4- + 4 H+	ZnSiO3	18.69	ZnSiO3 + 1 H2O -> 1 H2SiO4-2 + 1 Zn+2

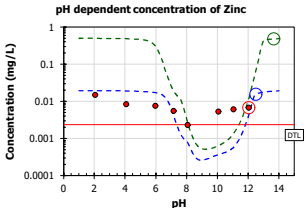

pH dependent concentration of Aluminum
pH dependent concentration of Arsenic
pH dependent concentration of Barium
pH dependent concentration of Calcium
pH dependent concentration of Cadmium
Al Profile at L/S=10.4 L/kg
As Profile at L/S=10.4 L/kg
Ba Profile at L/S=10.4 L/kg
Ca Profile at L/S=10.4 L/kg
Cd Profile at L/S=10.4 L/kg
pH dependent concentration of Chloride
pH dependent concentration of Cobalt
Inorganic Carbon
Cl Profile at L/S=10.4 L/kg
Co Profile at L/S=10.4 L/kg
CO32- Profile at L/S=10.4 L/kg
Cr Profile at L/S=10.4 L/kg
Cu Profile at L/S=10.4 L/kg
F Profile at L/S=10.4 L/kg
Fe Profile at L/S=10.4 L/kg
B Profile at L/S=10.4 L/kg
Si Profile at L/S=10.4 L/kg
Hg Profile at L/S=10.4 L/kg
Concentration (mg/L)
pH
DTL
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
Fluorite
Arsenocrandallite-therm
BaCaSO4[50%Ba]
CEM14_C3FS0.84H4.32
Cem07_C2ASH8
Cem07_Calcite
Hxyapatite[2]
CaCO3_BaCO3
CaCO3_SrCO3
Cem07_Calcite
LDH_Co_zc
LDH_Cu_zc
LDH_Mn_zc
LDH_Ni_zc
UO2CO3[s]
Co2SiO4
Albite[low]
Cem07_Al[OH]3[am]
Cem07_C2ASH8
FeAsO4:2H2O_am
Fe2[MoO4]3[2]
FeVO4:2H2O_am
Ferrihydrite
Strengite
Li2_CaO_Al2O3_SiO2_8H2O[s]
ZnSiO3

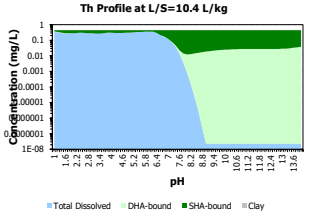

pH dependent concentration of Potassium
pH dependent concentration of Lithium
pH dependent concentration of Magnesium
pH dependent concentration of Manganese
pH dependent concentration of Molybdenum
K Profile at L/S=10.4 L/kg
Li Profile at L/S=10.4 L/kg
Mg Profile at L/S=10.4 L/kg
Mn Profile at L/S=10.4 L/kg
Mo Profile at L/S=10.4 L/kg
Total Dissolved
DHA-bound
SHA-bound
Clay
Carnotite
FeOxide
Li2_CaO_Al2O3_SiO2_8H2O[s]
AA_OH-hydrotalcite[cr]
LDH_Mn_zc
MnHPO4[C]
Fe2[MoO4]3[2]
Molybdocrandallite-exp
PbMoO4[c]
pH dependent concentration of Sodium
pH dependent concentration of Nickel
pH dependent concentration of Nitrate
pH dependent concentration of Lead
pH dependent concentration of Phosphate
Na Profile at L/S=10.4 L/kg
Ni Profile at L/S=10.4 L/kg
NO3 Profile at L/S=10.4 L/kg
Pb Profile at L/S=10.4 L/kg
PO4 Profile at L/S=10.4 L/kg
Albite[low]
LDH_Ni_zc
Ni[OH]2[s]
Ca2Pb[PO4]2
PbMoO4[c]
Pb[OH]2[C]
Hxyapatite[2]
MnHPO4[C]
Strengite
Sb Profile at L/S=10.4 L/kg
Se Profile at L/S=10.4 L/kg
Sn Profile at L/S=10.4 L/kg
SO4 Profile at L/S=10.4 L/kg
Sr Profile at L/S=10.4 L/kg
Ca[OH]2.Sn[OH]4
Sn[OH]2[s]
BaCaSO4[50%Ba]
CaCO3_SrCO3
Concentration (mg/L)
pH
D/L

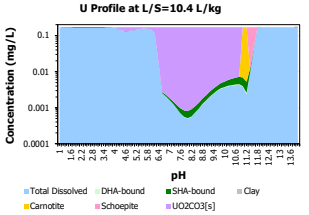

pH dependent concentration of Thorium
Concentration (mg/L)
pH
DTL

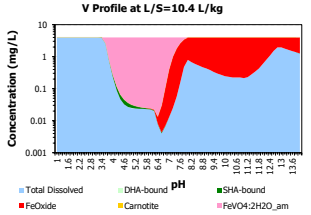

pH dependent concentration of Uranium
Concentration (mg/L)
pH
DTL

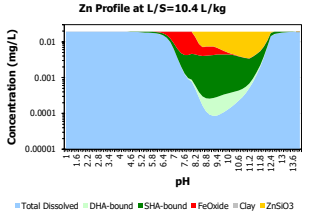

pH dependent concentration of Vanadium
Concentration (mg/L)
pH
DTL


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


Th Profile at L/S=10.4 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
Clay


U Profile at L/S=10.4 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
Clay
Carnotite
Schoepite
UO2CO3[s]


V Profile at L/S=10.4 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Carnotite
FeVO4:2H2O_am


Zn Profile at L/S=10.4 L/kg
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
ZnSiO3

Model Comparison: residuals - Concentration

Name **Red Mud**

Y Values Interpolation

Type Logarithmic

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*	*7*	*6*	*5*	*4*	*3*	*2*	*1*	*Total Avg*
pH	*2.04*	*4.07*	*5.97*	*7.15*	*8.06*	*10.1*	*11.0*	*12.0*	*Deviation*
Al	0.03	-0.34	0.50	-0.99	-1.31	-1.09	-0.89	-0.08	0.28
As	0.34	-2.42	-0.22	0.44	1.36	0.79	0.31	-0.04	0.37
Ba	0.03	0.13	1.55	-0.18	-0.30	-0.27	-0.24	-1.29	0.26
Br	-	-	-	-	-	-	-	-	-
Ca	0.03	0.36	0.74	-0.17	-0.17	0.36	0.45	-0.56	0.15
Cd	0.08	0.07	-0.02	-0.59	-1.21	-1.21	-1.19	-1.33	0.32
Cl	-0.05	0.05	0.02	0.01	-0.15	0.01	0.01	-0.03	0.02
Co	0.03	0.45	1.40	-0.30	-0.95	-0.55	0.40	0.96	0.27
CO32-	-	-	-	-	-	-	-	-	-
Cr	-0.03	-0.40	-0.19	-0.51	-1.09	0.35	0.77	0.77	0.21
Cu	0.03	0.83	1.34	-0.33	-0.63	-0.22	0.97	1.15	0.29
F	0.03	0.63	1.49	0.83	0.47	-0.30	-0.39	0.19	0.24
Fe	0.06	-1.16	-0.57	-0.63	0.04	-0.06	1.68	2.29	0.40
B	0.04	0.28	0.00	0.48	0.60	0.37	0.22	0.23	0.12
Si	0.03	-1.60	0.15	-0.28	-0.36	-0.63	-0.34	0.79	0.25
Hg	0.10	-0.94	-2.18	-0.87	-0.33	-0.01	0.03	0.03	0.32
K	-0.38	0.00	0.14	0.12	-0.04	0.03	0.02	-0.03	0.05
Li	0.03	0.37	0.78	1.00	1.08	0.88	1.33	0.41	0.30
Mg	0.03	0.35	1.59	0.98	1.46	0.83	-0.74	-2.26	0.43
Mn	0.03	0.31	0.39	0.51	2.15	-1.04	-1.02	-1.47	0.38
Mo	2.16	-1.44	0.89	0.42	-0.02	0.03	0.02	-0.03	0.35
Na	-0.09	-0.05	-0.02	0.00	-0.01	0.00	-0.01	-0.08	0.02
Ni	0.03	0.29	1.28	-0.34	0.14	-0.50	-0.17	0.30	0.19
NO3	0.43	0.43	0.43	0.43	0.43	0.43	0.43	-1.92	0.28
Pb	2.68	2.13	-0.41	-0.35	0.30	0.02	0.15	1.61	0.48
PO4	0.61	-0.36	2.58	1.70	1.34	-0.18	-2.60	-2.06	0.60
Sb	0.27	0.27	0.00	0.27	0.27	0.27	0.27	0.27	0.09
Se	0.28	0.36	0.33	0.03	0.13	0.06	0.01	-0.03	0.07
Sn	0.70	-1.67	0.23	0.23	0.85	0.62	0.61	-0.16	0.28
SO4	0.03	0.23	0.61	0.40	0.20	0.29	0.28	0.27	0.12
Sr	0.03	0.35	0.97	-0.37	-0.27	0.38	0.80	-0.20	0.18
Th	-0.17	0.30	1.85	1.28	0.39	0.67	0.76	0.66	0.33
U	0.01	0.60	2.23	0.20	-0.21	0.65	0.63	2.30	0.42
V	0.03	0.04	0.90	0.62	1.53	-0.40	-0.82	-0.58	0.27
Zn	0.11	0.35	0.35	-0.12	-0.47	-1.16	-1.02	-0.19	0.21
Avg Deviati	0.11	0.15	0.19	0.11	0.14	0.10	0.14	0.18	0.26

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