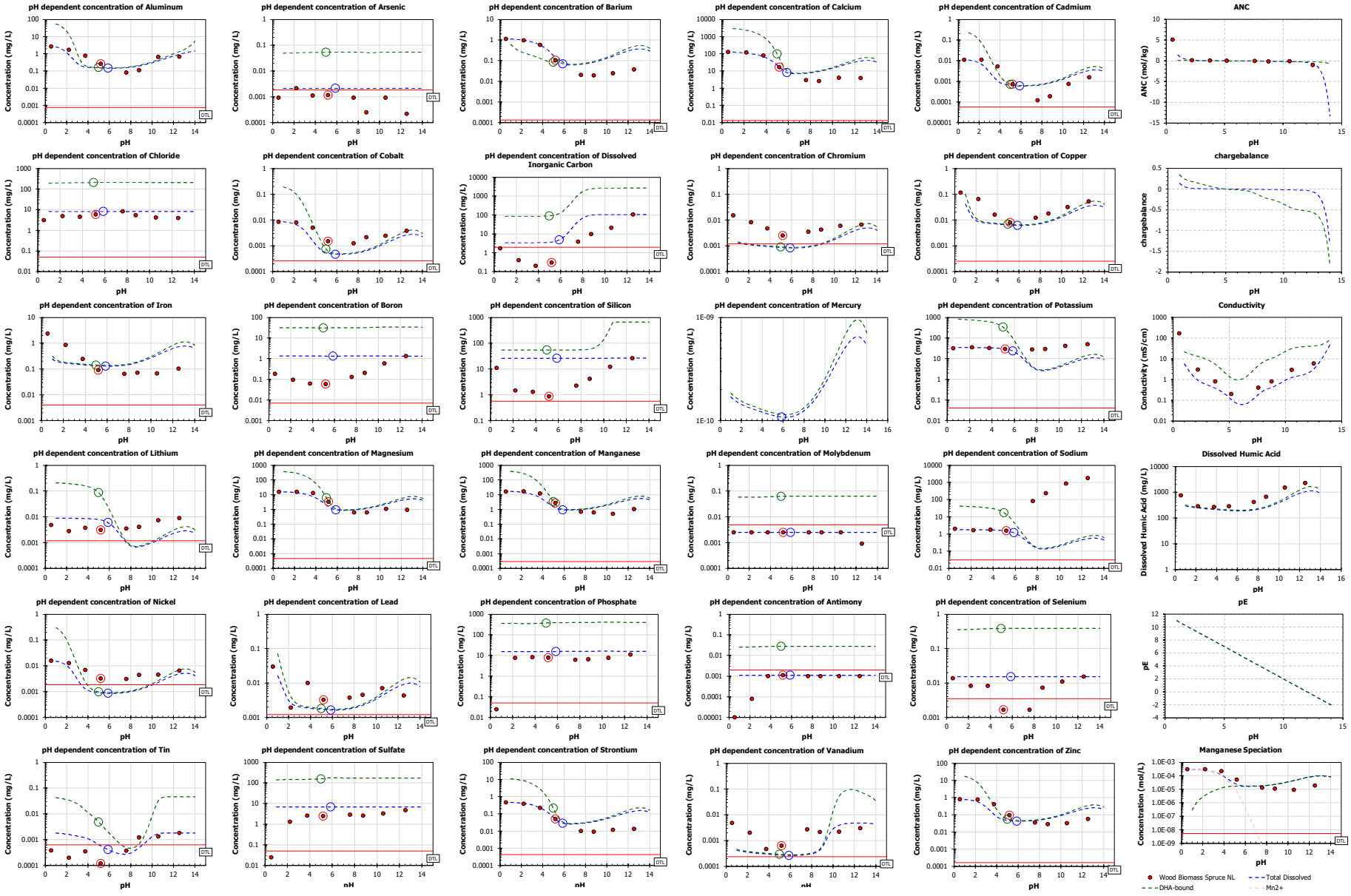
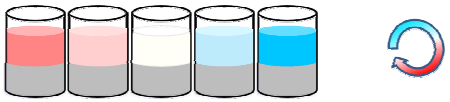
WOOD BIOMASS SPRUCE NL

COMPARISON pH DEPENDENCE WITH MODEL



Object pH Dependent Leaching Test Model
Name Wood Biomass Spruce NL

pH Dependent Leaching Test Scenario



Lab Test

Extra L/S Simulation

Lab Test

Model Parameters

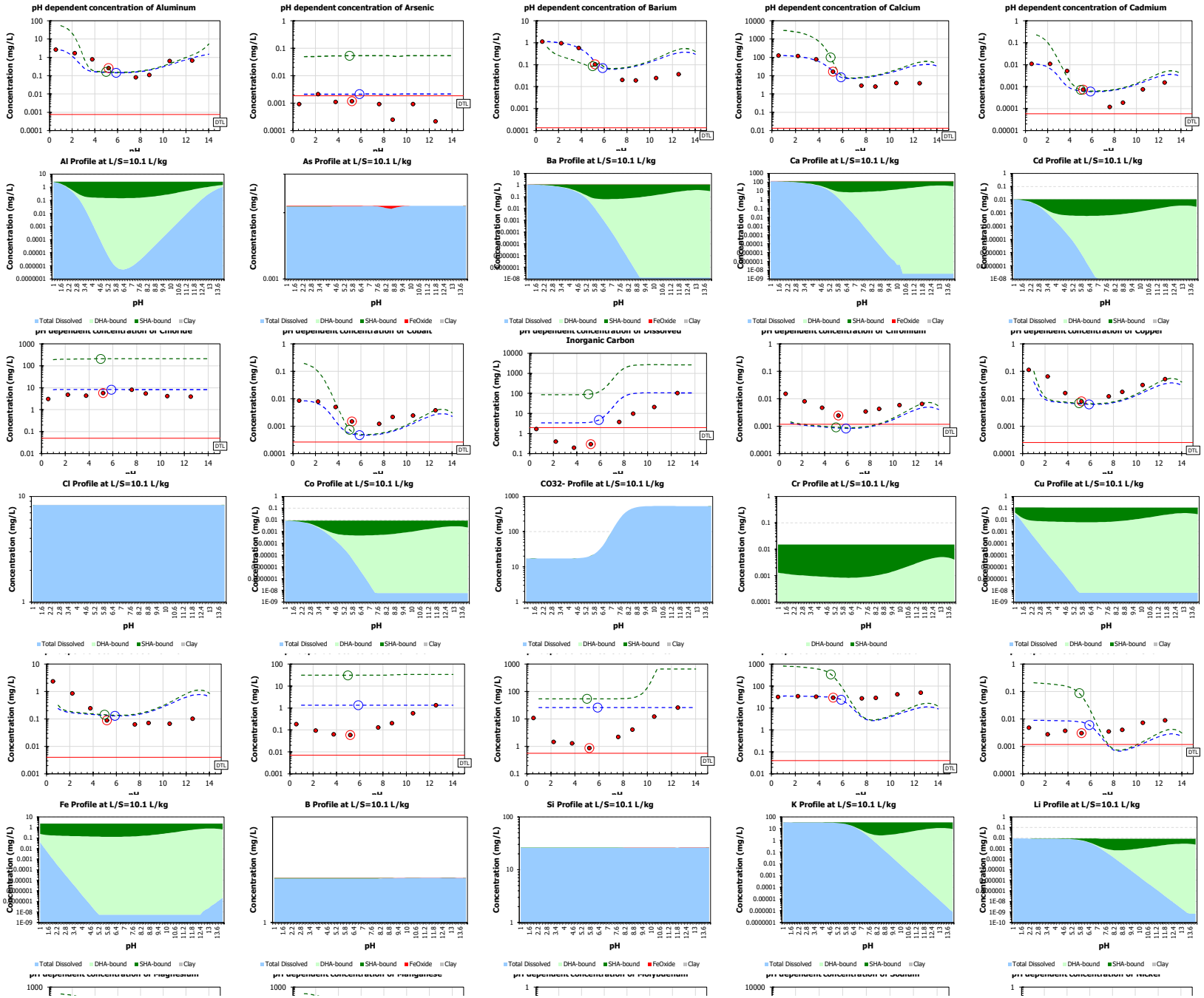
Entity	Unit	Default
c0		-3.686
c1		-0.2018
c2		0.07175
c3		-0.01493
c4		0.001458
c5		-4.822E-05
Clay	mg/kg	3000
Hydrous Ferric Oxide	mg/kg	30.00
L/S	L/kg	10.12
pE		6.820
pH		5.180
Solid Humic Acid	mg/kg	3.500E+04
Simulated Low L/S	L/kg	0.4000

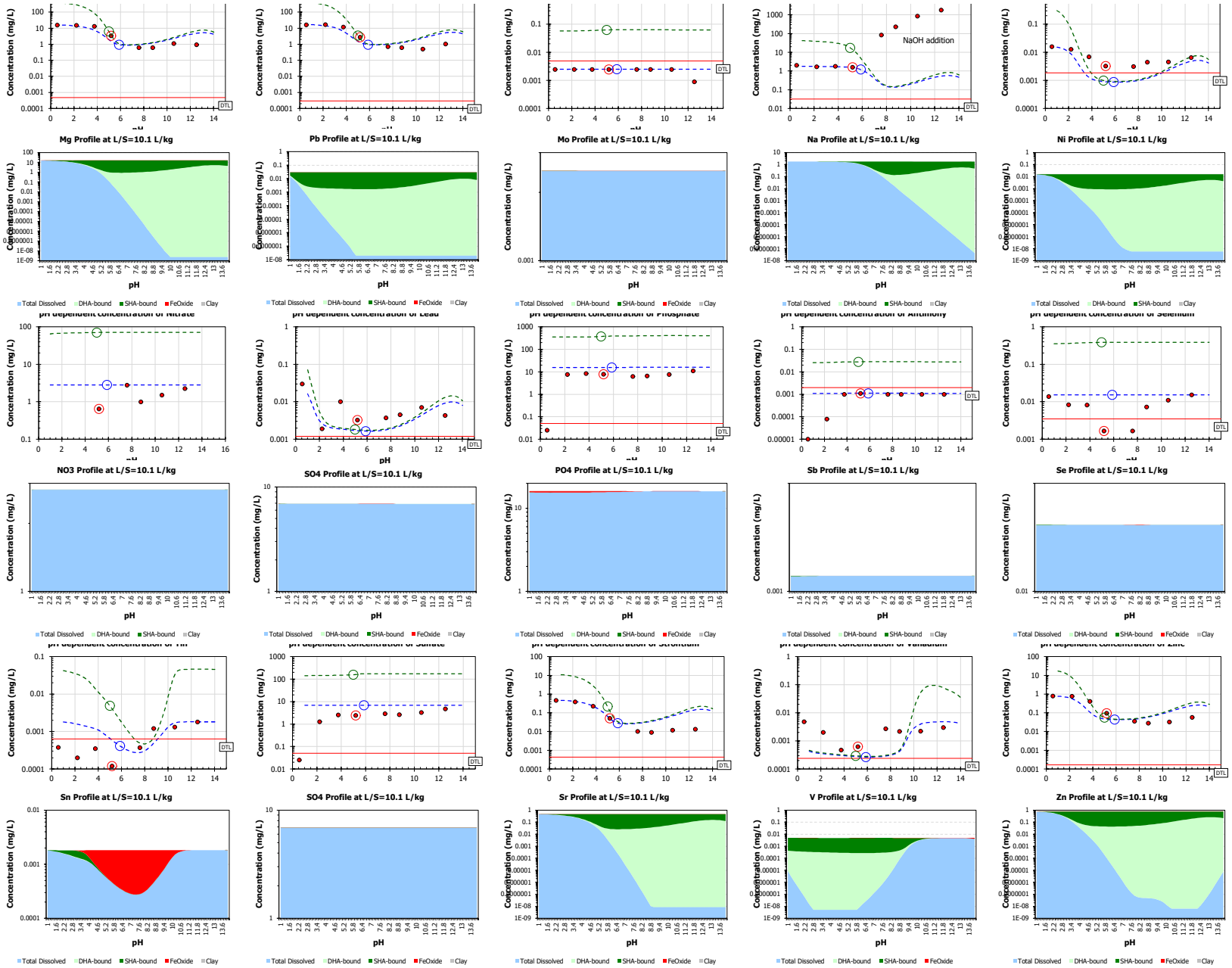
Available Content

Entity	mg/kg	Entity	mg/kg	Entity	mg/kg
Al	27.05	B	13.56	PO4	162.7
As	0.02177	Si	265.2	Sb	0.01118
Ba	11.56	Hg	2.006E-08	Se	0.1552
Ca	1297	K	356.1	Sn	0.01840
Cd	0.1116	Li	0.09090	SO4	69.84
Cl	83.88	Mg	161.4	Sr	4.761
Co	0.08724	Mn	170.0	V	0.04941
CO32-	5394	Mo	0.02525	Zn	7.991
Cr	0.1540	Na	18.22		
Cu	1.156	Ni	0.1604		
F	1.900E-09	NO3	28.47		
Fe	24.05	Pb	0.3045		

Minerals

Name	> 1E-13 mol/kg	Log(K)	Reaction
AA_Fe[OH]3[am]		16.60	AA_Fe[OH]3[am] + 1 H2O -> 1 Fe[OH]4- + 1 H+
AA_Fe[OH]3[microcr]		18.60	AA_Fe[OH]3[microcr] + 1 H2O -> 1 Fe[OH]4- + 1 H+
AA_Silica[am]	Yes	24.33	AA_Silica[am] + 2 H2O -> 2 H+ + 1 H2SiO4-2
alpha-TCP		25.50	alpha-TCP -> 3 Ca+2 + 2 PO4-3
Anorthite		63.81	Anorthite + 8 H2O -> 2 Al[OH]4- + 1 Ca+2 + 4 H+ + 2 H2SiO4-2
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
Barite	Yes	9.976	Barite -> 1 Ba+2 + 1 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[Sb[OH]6]2[sAJ]		12.55	Ca[Sb[OH]6]2[sAJ] -> 1 Ca+2 + 2 Sb[OH]6-
Ca[Sb[OH]6]2[sC]		9.942	Ca[Sb[OH]6]2[sC] -> 1 Ca+2 + 2 Sb[OH]6-
Ca2Cd[PO4]2		32.95	Ca2Cd[PO4]2 -> 2 Ca+2 + 1 Cd+2 + 2 PO4-3
Ca3[AsO4]2:2.25H2O		21.14	Ca3[AsO4]2:2.25H2O -> 2 AsO4-3 + 3 Ca+2 + 2.25 H2O
Ca3[AsO4]2:6H2O		18.89	Ca3[AsO4]2:6H2O -> 2 AsO4-3 + 3 Ca+2 + 6 H2O
Ca4[OH]2[AsO4]2:4H2O[c]		-0.5010	Ca4[OH]2[AsO4]2:4H2O[c] + 2 H+ -> 2 AsO4-3 + 4 Ca+2 + 6 H2O
Ca4Cd[PO4]3OH		39.23	Ca4Cd[PO4]3OH + 1 H+ -> 4 Ca+2 + 1 Cd+2 + 1 H2O + 3 PO4-3
Ca5[OH][AsO4]3[c]		26.13	Ca5[OH][AsO4]3[c] + 1 H+ -> 3 AsO4-3 + 5 Ca+2 + 1 H2O
Carnotite		-3.015	Carnotite + 4 H+ + 1 e- -> 2 H2O + 1 K+ + 1 UO2+ + 1 VO2+
CaSeO3:2H2O		-2.814	CaSeO3:2H2O -> 1 Ca+2 + 2 H+ + 1 H2O + 1 SeO4-2 + 2 e-
CaSeO4:2H2O		3.020	CaSeO4:2H2O -> 1 Ca+2 + 2 H2O + 1 SeO4-2
Cd[OH]2[C]		-13.65	Cd[OH]2[C] + 2 H+ -> 1 Cd+2 + 2 H2O
Cem07_Al[OH]3[am]		13.76	Cem07_Al[OH]3[am] + 1 H2O -> 1 Al[OH]4- + 1 H+
Cem07_Al2O3		26.36	Cem07_Al2O3 + 5 H2O -> 2 Al[OH]4- + 2 H+
Cem07_Anhydrite		4.360	Cem07_Anhydrite -> 1 Ca+2 + 1 SO4-2
Cem07_Brucite		-16.83	Cem07_Brucite + 2 H+ -> 2 H2O + 1 Mg+2
Cem07_C2AH8		-14.43	Cem07_C2AH8 + 2 H+ -> 2 Al[OH]4- + 2 Ca+2 + 5 H2O
Cem07_C2ASH8		17.40	Cem07_C2ASH8 -> 2 Al[OH]4- + 2 Ca+2 + 3 H2O + 1 H2SiO4-2
Cem07_C2FH8		-10.39	Cem07_C2FH8 + 2 H+ -> 2 Ca+2 + 2 Fe[OH]4- + 5 H2O
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_C4AH13		-58.57	Cem07_C4AH13 + 6 H+ -> 2 Al[OH]4- + 4 Ca+2 + 12 H2O
Cem07_C4FH13		-54.57	Cem07_C4FH13 + 6 H+ -> 4 Ca+2 + 2 Fe[OH]4- + 12 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
Cem07_Portlandite		-22.79	Cem07_Portlandite + 2 H+ -> 1 Ca+2 + 2 H2O
Cem07_Syngenite		-7.200	Cem07_Syngenite -> 1 Ca+2 + 1 H2O + 2 K+ + 2 SO4-2
Cr[OH]3[A]		68.13	Cr[OH]3[A] + 1 H2O -> 1 CrO4-2 + 5 H+ + 3 e-
Fe_Vanadate		19.18	Fe_Vanadate + 1 H2O -> 0.5 Fe[OH]4- + 1 VO2+ + 0.5 e-
Fluorite		10.96	Fluorite -> 1 Ca+2 + 2 F-
Larnite		-17.52	Larnite + 2 H+ -> 2 Ca+2 + 1 H2SiO4-2
Laumontite-exp		116.0	Laumontite-exp + 8 H2O -> 2 Al[OH]4- + 1 Ca+2 + 8 H+ + 4 H2SiO4-2
MINTEQ_Albite[low]		85.27	MINTEQ_Albite[low] + 8 H2O -> 1 Al[OH]4- + 6 H+ + 3 H2SiO4-2 + 1 Na+
Ni[OH]2[s]		-10.80	Ni[OH]2[s] + 2 H+ -> 2 H2O + 1 Ni+2
Pb[OH]2[C]		-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
Pb2V2O7		0.9500	Pb2V2O7 + 3 H+ -> 1.5 H2O + 1 Pb+2 + 1 VO2+
Pb3[VO4]2		-3.070	Pb3[VO4]2 + 4 H+ -> 2 H2O + 1.5 Pb+2 + 1 VO2+
PbMoO4[c]		15.80	PbMoO4[c] -> 1 MoO4-2 + 1 Pb+2
Sb[OH]3[s]		32.89	Sb[OH]3[s] + 3 H2O -> 3 H+ + 1 Sb[OH]6- + 2 e-
Strengite		48.00	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
ThF4:2.5H2O		31.86	ThF4:2.5H2O -> 4 F- + 2.5 H2O + 1 Th+4
Tyuyamunite		-4.825	Tyuyamunite + 4 H+ + 1 e- -> 0.5 Ca+2 + 2 H2O + 1 UO2+ + 1 VO2+
Wairakite		113.6	Wairakite + 10 H2O -> 2 Al[OH]4- + 1 Ca+2 + 8 H+ + 4 H2SiO4-2
Willemite		6.289	Willemite + 2 H+ -> 1 H2SiO4-2 + 2 Zn+2
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=10.1 L/kg
As Profile at L/S=10.1 L/kg
Ba Profile at L/S=10.1 L/kg
Ca Profile at L/S=10.1 L/kg
Cd Profile at L/S=10.1 L/kg
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
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=10.1 L/kg
Co Profile at L/S=10.1 L/kg
CO32- Profile at L/S=10.1 L/kg
Cr Profile at L/S=10.1 L/kg
Cu Profile at L/S=10.1 L/kg
Fe Profile at L/S=10.1 L/kg
B Profile at L/S=10.1 L/kg
Si Profile at L/S=10.1 L/kg
K Profile at L/S=10.1 L/kg
Li Profile at L/S=10.1 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


Mg Profile at L/S=10.1 L/kg
Pb Profile at L/S=10.1 L/kg
Mo Profile at L/S=10.1 L/kg
Na Profile at L/S=10.1 L/kg
NaOH addition
Ni Profile at L/S=10.1 L/kg
NO3 Profile at L/S=10.1 L/kg
SO4 Profile at L/S=10.1 L/kg
PO4 Profile at L/S=10.1 L/kg
Sb Profile at L/S=10.1 L/kg
Se Profile at L/S=10.1 L/kg
Sn Profile at L/S=10.1 L/kg
SO4 Profile at L/S=10.1 L/kg
Sr Profile at L/S=10.1 L/kg
V Profile at L/S=10.1 L/kg
Zn Profile at L/S=10.1 L/kg
Concentration (mg/L)
pH
DTL
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay

Model Comparison: residuals - Concentration

Name **Wood Biomass Spruce 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*	*7*	*6*	*5*	*4*	*3*	*2*	*1*	*Total Avg*
pH	*0.550*	*2.21*	*3.75*	*5.18*	*7.58*	*8.76*	*10.6*	*12.5*	*Deviation*
Al	-0.03	-0.28	-0.66	-0.24	0.29	0.25	-0.22	0.14	0.11
As	0.36	0.00	0.28	0.26	0.36	0.92	0.37	0.99	0.19
Ba	0.00	0.01	0.00	0.12	0.51	0.64	0.83	0.97	0.19
Ca	0.00	-0.04	-0.06	0.02	0.41	0.57	0.67	1.00	0.17
Cd	-0.01	-0.21	-0.70	-0.07	0.74	0.64	0.33	0.34	0.16
Cl	0.42	0.23	0.27	0.15	0.00	0.18	0.30	0.32	0.09
Co	0.00	-0.08	-0.51	-0.46	-0.39	-0.53	-0.29	-0.16	0.13
CO32-	-	-	-	-	-	-	-	-	-
Cr	-1.03	-0.88	-0.70	-0.46	-0.59	-0.57	-0.43	-0.15	0.23
Cu	-0.44	-0.87	-0.36	-0.10	-0.26	-0.32	-0.28	-0.17	0.15
Fe	-0.86	-0.70	-0.23	0.17	0.34	0.39	0.71	0.85	0.21
B	0.86	1.15	1.33	1.36	1.01	0.82	0.36	0.00	0.34
Si	0.37	1.25	1.30	1.48	1.07	0.80	0.33	0.00	0.34
Hg	-	-	-	-	-	-	-	-	-
K	0.04	-0.01	0.01	0.01	-0.85	-1.04	-0.92	-0.68	0.22
Li	0.26	0.50	0.36	0.40	-0.54	-0.77	-0.76	-0.52	0.19
Mg	0.00	-0.05	-0.25	-0.33	0.18	0.28	0.32	0.71	0.12
Mn	0.00	-0.07	-0.28	-0.33	0.15	0.31	0.69	0.69	0.14
Mo	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.44	0.06
Na	-0.05	0.02	-0.02	-0.01	-2.62	-3.23	-3.53	-3.52	0.81
Ni	-0.02	-0.17	-0.73	-0.56	-0.52	-0.57	-0.29	-0.13	0.16
NO3	-	-	-	0.64	0.00	0.45	0.27	0.10	0.17
Pb	-0.26	0.14	-0.73	-0.28	-0.32	-0.30	-0.21	0.33	0.13
PO4	2.79	0.31	0.27	0.30	0.40	0.39	0.33	0.16	0.36
Sb	2.04	1.14	0.04	0.00	0.04	0.04	0.04	0.04	0.29
Se	0.04	0.27	0.27	0.96	0.96	0.32	0.14	0.00	0.18
Sn	0.68	0.90	0.53	0.69	-0.13	-0.39	0.11	0.00	0.19
SO4	2.44	0.73	0.43	0.45	0.38	0.42	0.32	0.16	0.34
Sr	0.00	0.02	0.01	-0.01	0.44	0.59	0.76	1.03	0.18
V	-1.01	-0.77	-0.19	-0.36	-0.97	-0.70	0.26	0.20	0.23
Zn	-0.01	-0.14	-0.59	-0.32	0.12	0.32	0.54	0.62	0.14
Avg Deviati	0.17	0.11	0.10	0.10	0.13	0.15	0.15	0.15	0.21

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