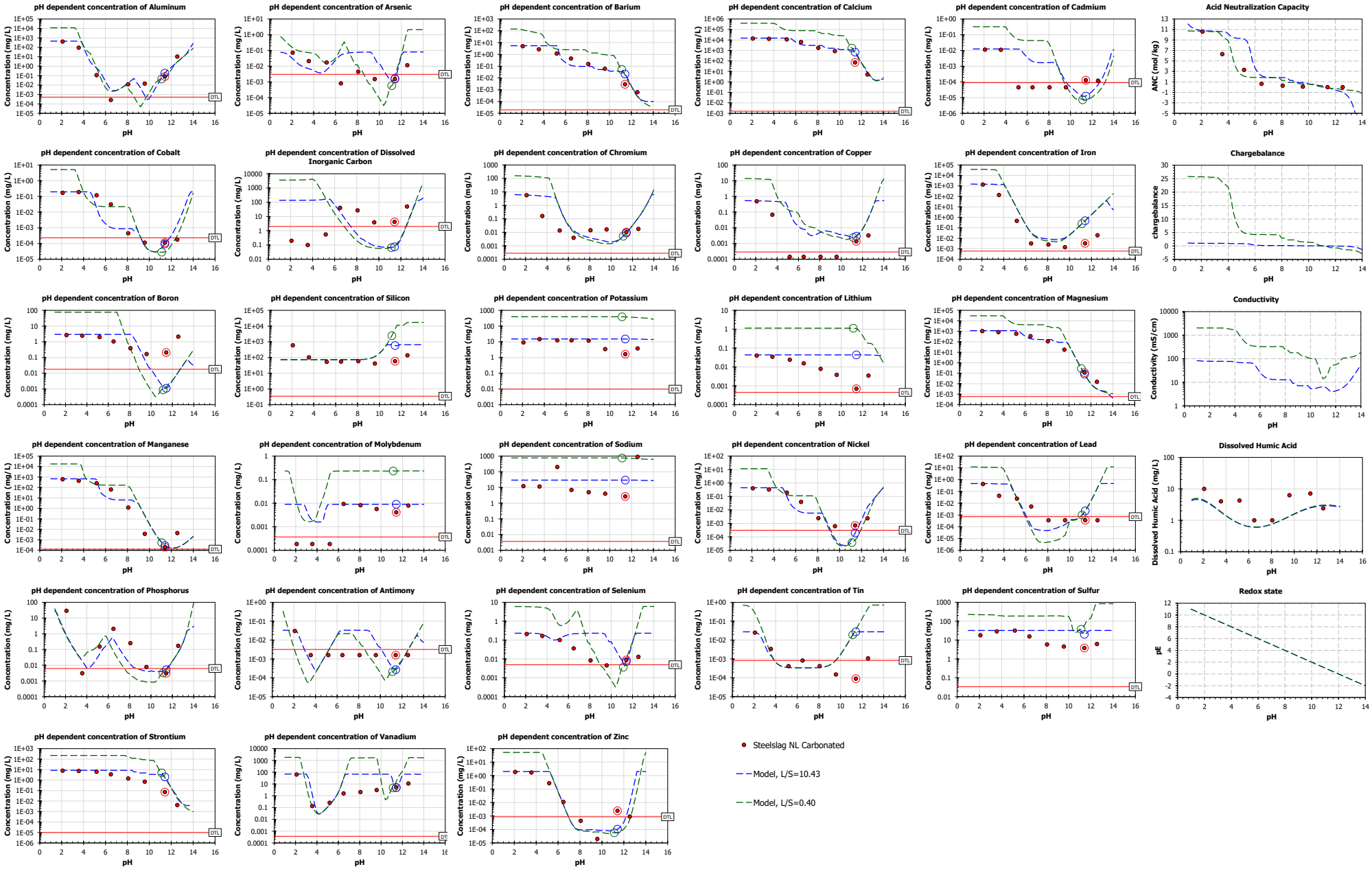
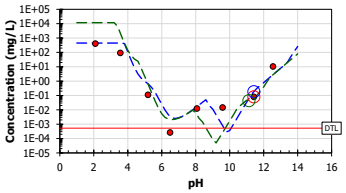
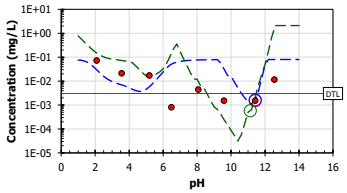
COMPARISON pH DEPENDENCE DATA WITH MODEL



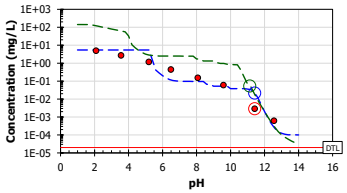
pH dependent concentration of Aluminum



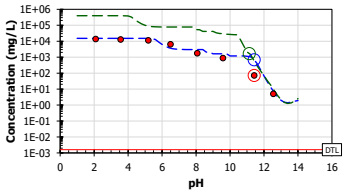
pH dependent concentration of Arsenic



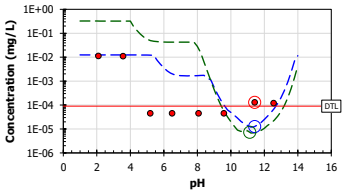
pH dependent concentration of Barium



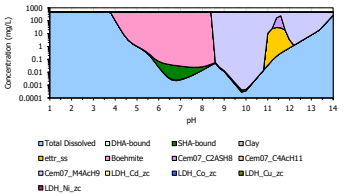
pH dependent concentration of Calcium



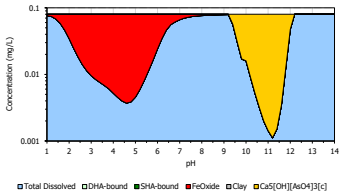
pH dependent concentration of Cadmium



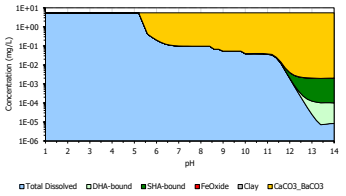
Al Profile at L/S=10.4 L/kg



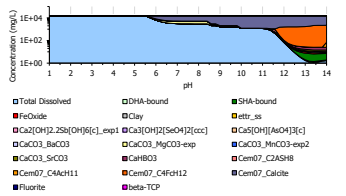
As Profile at L/S=10.4 L/kg



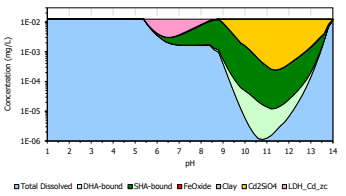
Ba Profile at L/S=10.4 L/kg



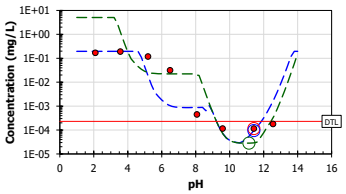
Ca Profile at L/S=10.4 L/kg



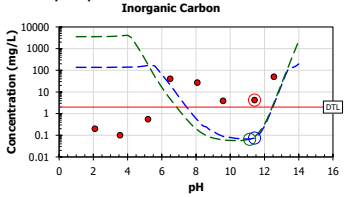
Cd Profile at L/S=10.4 L/kg



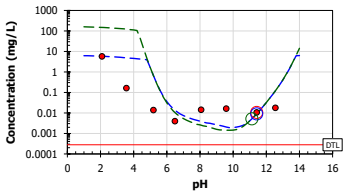
pH dependent concentration of Cobalt



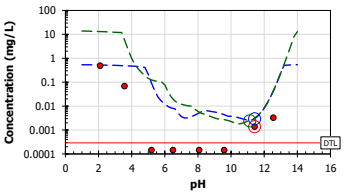
pH dependent concentration of Dissolved Inorganic Carbon



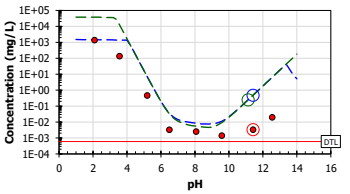
pH dependent concentration of Chromium



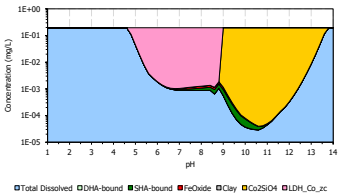
pH dependent concentration of Copper



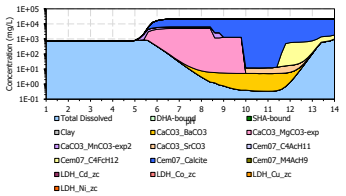
pH dependent concentration of Iron



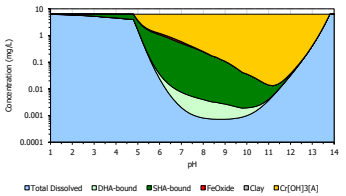
Co Profile at L/S=10.4 L/kg



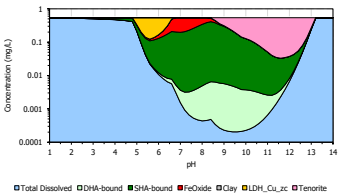
CO32- Profile at L/S=10.4 L/kg



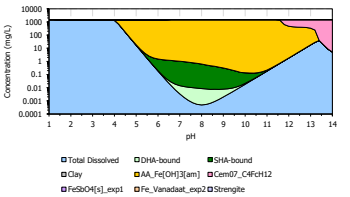
Cr Profile at L/S=10.4 L/kg



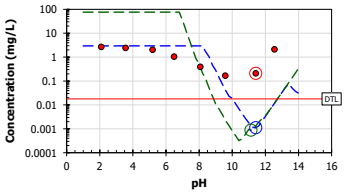
Cu Profile at L/S=10.4 L/kg



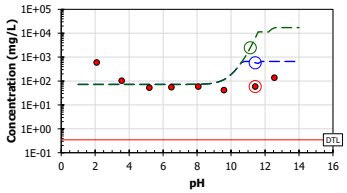
Fe Profile at L/S=10.4 L/kg



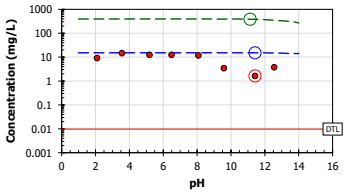
pH dependent concentration of Boron



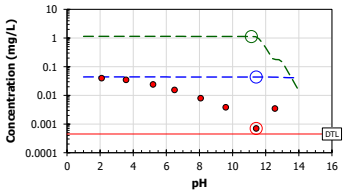
pH dependent concentration of Silicon



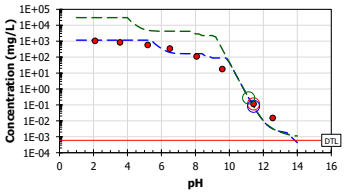
pH dependent concentration of Potassium



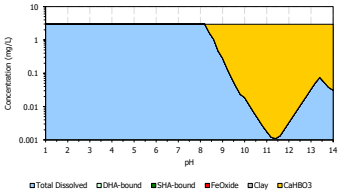
pH dependent concentration of Lithium



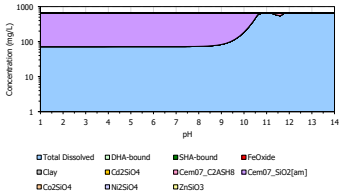
pH dependent concentration of Magnesium



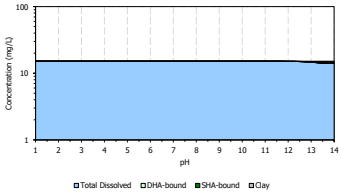
B Profile at L/S=10.4 L/kg



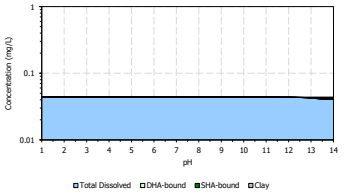
Si Profile at L/S=10.4 L/kg



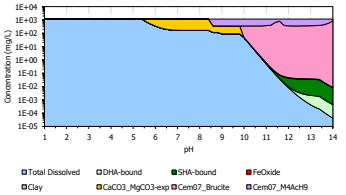
K Profile at L/S=10.4 L/kg



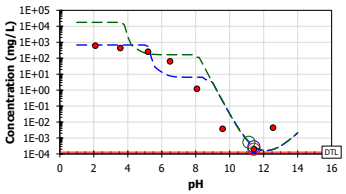
Li Profile at L/S=10.4 L/kg



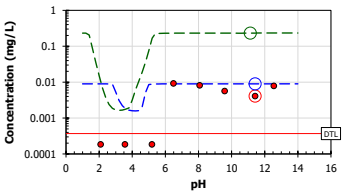
Mg Profile at L/S=10.4 L/kg



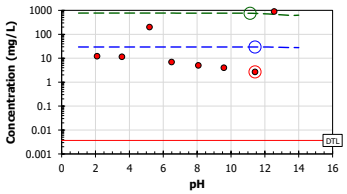
pH dependent concentration of Manganese



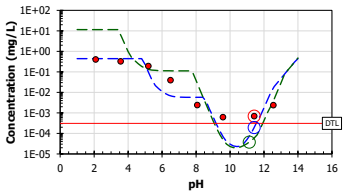
pH dependent concentration of Molybdenum



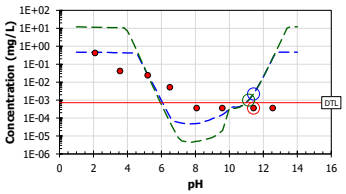
pH dependent concentration of Sodium



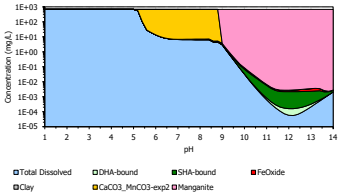
pH dependent concentration of Nickel



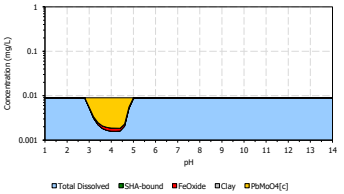
pH dependent concentration of Lead



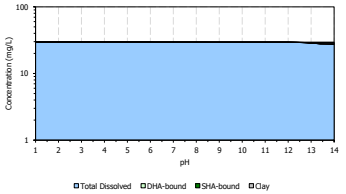
Mn Profile at L/S=10.4 L/kg



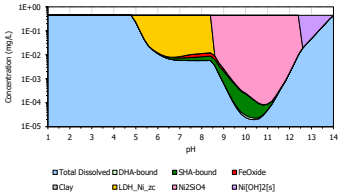
Mo Profile at L/S=10.4 L/kg



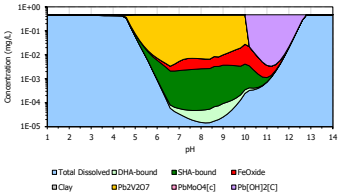
Na Profile at L/S=10.4 L/kg



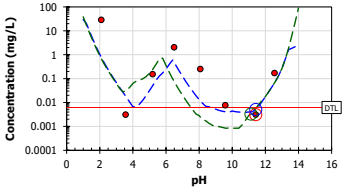
Ni Profile at L/S=10.4 L/kg



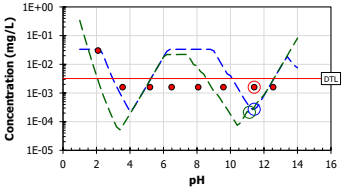
Pb Profile at L/S=10.4 L/kg



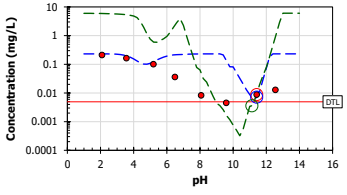
pH dependent concentration of Phosphorus



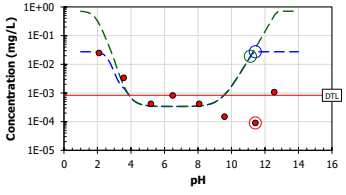
pH dependent concentration of Antimony



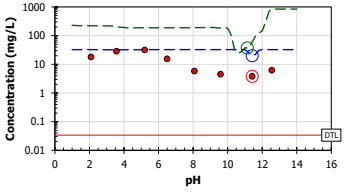
pH dependent concentration of Selenium



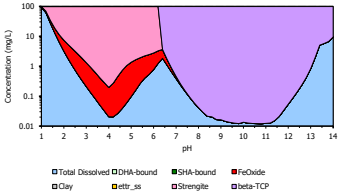
pH dependent concentration of Tin



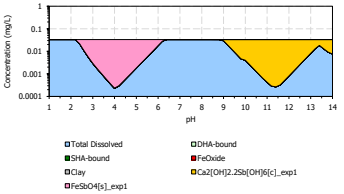
pH dependent concentration of Sulfur



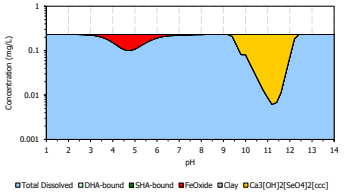
PO4 Profile at L/S=10.4 L/kg



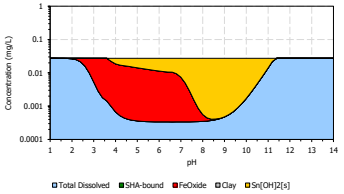
Sb Profile at L/S=10.4 L/kg



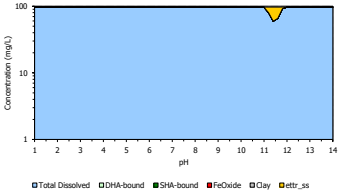
Se Profile at L/S=10.4 L/kg



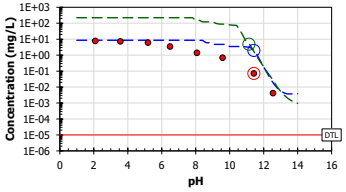
Sn Profile at L/S=10.4 L/kg



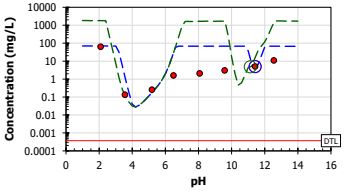
SO4 Profile at L/S=10.4 L/kg



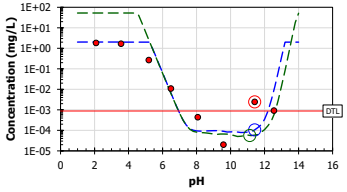
pH dependent concentration of Strontium



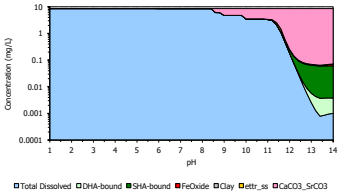
pH dependent concentration of Vanadium



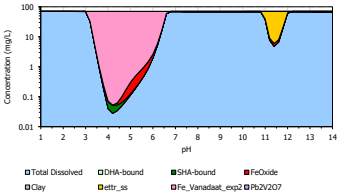
pH dependent concentration of Zinc



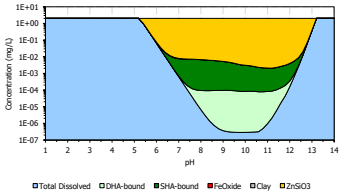
Sr Profile at L/S=10.4 L/kg



V Profile at L/S=10.4 L/kg



Zn Profile at L/S=10.4 L/kg



Name **Steelslag NL carbonated**

pH Dependent Leaching Test Scenario

Lab Test

Extra L/S Simulation

Lab Test

Model Parameters

Entity	Unit	Default
c0		-6.084
c1		0.7171
c2		-0.3539
c3		0.05510
c4		-0.003451
c5		7.607E-05
Clay	mg/kg	3000
Hydrous Ferric Oxid	mg/kg	500.0
L/S	L/kg	10.43
pE		0.2000
pH		11.80
Solid Humic Acid	mg/kg	598.0
Simulated Low L/S	L/kg	0.4000

Available Content

Entity	Unit	Default	Entity	Unit	Default	Entity	Unit	Default
Acetic acid	mg/kg	2.220E-07	F	mg/kg	10.00	Pb	mg/kg	4.871
Ag	mg/kg	1.079E-07	Fe	mg/kg	1.573E+04	PO4	mg/kg	1016
Al	mg/kg	4689	B	mg/kg	30.80	Sb	mg/kg	0.3464
As	mg/kg	0.8354	Si	mg/kg	6864	Se	mg/kg	2.407
Ba	mg/kg	56.84	Hg	mg/kg	2.006E-07	Sn	mg/kg	0.2850
Br	mg/kg	7.990E-08	K	mg/kg	158.0	SO4	mg/kg	1011
Ca	mg/kg	1.587E+05	Li	mg/kg	0.4571	Sr	mg/kg	89.37
Cd	mg/kg	0.1299	Mg	mg/kg	1.211E+04	Th	mg/kg	2.320E-07
Cl	mg/kg	15.00	Mn	mg/kg	7043	U	mg/kg	2.380E-07
Co	mg/kg	2.036	Mo	mg/kg	0.09358	V	mg/kg	731.0
CO32-	mg/kg	2.230E+05	Na	mg/kg	308.1	Zn	mg/kg	21.03
Cr	mg/kg	65.62	Ni	mg/kg	4.627			
Cu	mg/kg	5.644	NO3	mg/kg	6.200E-08			

Solid Solutions

Name	End Member	Log(K)	Reaction
ettr_ss	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
	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	-46.87	BO3_Ettringite_ss + 7 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 H2BO3- + 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
	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_Fe[OH]3[am]	Yes	16.60	AA_Fe[OH]3[am] + 1 H2O -> 1 Fe[OH]4- + 1 H+
Antimocrandallite-e	Yes	63.00	Antimocrandallite-exp + 8 H2O -> 3 Al[OH]4- + 1 Ca+2 + 3 H+ + 2 Sb[OH]6-
Ba[SCr]O4[96%SO4]	Yes	9.790	Ba[SCr]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2
beta-TCP	Yes	28.93	beta-TCP -> 3 Ca+2 + 2 PO4-3
Boehmite	Yes	14.42	Boehmite + 2 H2O -> 1 Al[OH]4- + 1 H+
Ca2[OH]2.2Sb[OH]6	Yes	5.000	Ca2[OH]2.2Sb[OH]6[c]_exp1 + 2 H+ -> 2 Ca+2 + 2 H2O + 2 Sb[OH]6-
Ca3[OH]2[SeO4]2[c	Yes	6.477	Ca3[OH]2[SeO4]2[ccc] + 2 H+ -> 3 Ca+2 + 2 H2O + 2 SeO4-2
Ca5[OH][AsO4]3[c]	Yes	26.13	Ca5[OH][AsO4]3[c] + 1 H+ -> 3 AsO4-3 + 5 Ca+2 + 1 H2O
CaCO3_BaCO3	Yes	22.00	CaCO3_BaCO3 -> 1 Ba+2 + 2 CO3-2 + 1 Ca+2
CaCO3_Li2CO3	Yes	21.30	CaCO3_Li2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 Li+
CaCO3_MgCO3-exp	Yes	18.02	CaCO3_MgCO3-exp -> 2 CO3-2 + 1 Ca+2 + 1 Mg+2
CaCO3_MnCO3-exp	Yes	19.78	CaCO3_MnCO3-exp2 -> 2 CO3-2 + 1 Ca+2 + 1 Mn+2
CaCO3_SrCO3	Yes	19.85	CaCO3_SrCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Sr+2
CaHBO3	Yes	-2.097	CaHBO3 + 1 H+ -> 1 Ca+2 + 1 H2BO3-
Cd2SiO4	Yes	6.059	Cd2SiO4 + 2 H+ -> 2 Cd+2 + 1 H2SiO4-2
Cem07_Brucite	Yes	-16.83	Cem07_Brucite + 2 H+ -> 2 H2O + 1 Mg+2
Cem07_C2ASH8	Yes	17.40	Cem07_C2ASH8 -> 2 Al[OH]4- + 2 Ca+2 + 3 H2O + 1 H2SiO4-2
Cem07_C4AcH11	Yes	-24.50	Cem07_C4AcH11 + 4 H+ -> 2 Al[OH]4- + 1 CO3-2 + 4 Ca+2 + 9 H2O
Cem07_C4FcH12	Yes	-20.47	Cem07_C4FcH12 + 4 H+ -> 1 CO3-2 + 4 Ca+2 + 2 Fe[OH]4- + 10 H2O
Cem07_C4FsH12	Yes	-22.77	Cem07_C4FsH12 + 4 H+ -> 4 Ca+2 + 2 Fe[OH]4- + 10 H2O + 1 SO4-2
Cem07_Calcite	Yes	8.485	Cem07_Calcite -> 1 CO3-2 + 1 Ca+2
Cem07_Gypsum	Yes	4.583	Cem07_Gypsum -> 1 Ca+2 + 2 H2O + 1 SO4-2
Cem07_M4AcH9	Yes	-4.823	Cem07_M4AcH9 + 4 H+ -> 2 Al[OH]4- + 1 CO3-2 + 7 H2O + 4 Mg+2
Cem07_SiO2[am]	Yes	24.21	Cem07_SiO2[am] + 2 H2O -> 2 H+ + 1 H2SiO4-2
Co2SiO4	Yes	5.289	Co2SiO4 + 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-
Fe_Vanadaat_exp2	Yes	20.48	Fe_Vanadaat_exp2 + 2 H2O -> 1 Fe[OH]4- + 1 VO2+
FeSbO4[s]_exp1	Yes	32.48	FeSbO4[s]_exp1 + 6 H2O -> 1 Fe[OH]4- + 2 H+ + 1 Sb[OH]6-
Fluorite	Yes	10.96	Fluorite -> 1 Ca+2 + 2 F-
LDH_Cd_zc	Yes	60.06	LDH_Cd_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 3 Cd+2 + 1 H+
LDH_Co_zc	Yes	60.01	LDH_Co_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 3 Co+2 + 1 H+
LDH_Cu_zc	Yes	58.21	LDH_Cu_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 3 Cu+2 + 1 H+
LDH_Ni_zc	Yes	57.91	LDH_Ni_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 1 H+ + 3 Ni+2
Li2_CaO_Al2O3_SiO2_8H2O[s]	Yes	22.69	Li2_CaO_Al2O3_SiO2_8H2O[s] -> 2 Al[OH]4- + 1 Ca+2 + 3 H2O + 1 H2SiO4-2 + 2 Li+
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
Ni2SiO4	Yes	5.498	Ni2SiO4 + 2 H+ -> 1 H2SiO4-2 + 2 Ni+2
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+
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
Spodumene2	Yes	58.00	Spodumene2 + 6 H2O -> 1 Al[OH]4- + 4 H+ + 2 H2SiO4-2 + 1 Li+
Strengite	Yes	48.00	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
Tenorite	Yes	-7.644	Tenorite + 2 H+ -> 1 Cu+2 + 1 H2O
ZnSiO3	Yes	18.69	ZnSiO3 + 1 H2O -> 1 H2SiO4-2 + 1 Zn+2

Model Comparison: residuals - Concentration

Sample

Name **Steelslag NL Carbonated**

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	*8*	*7*	*6*	*5*	*4*	*3*	*2*	*1*	*Total Avg*
pH	*2.09*	*3.56*	*5.19*	*6.49*	*8.07*	*9.58*	*11.4*	*12.6*	*Deviation*
Al	0.04	0.69	0.76	1.13	0.13	-1.26	0.36	-0.57	0.26
As	-0.39	-0.48	-0.47	1.79	1.24	1.33	0.03	0.84	0.35
Ba	0.04	0.30	0.67	-0.58	-0.20	-0.07	0.87	-0.36	0.17
Ca	0.04	0.07	0.13	-0.25	0.23	0.27	0.98	0.16	0.14
Cd	0.04	0.05	2.43	1.66	1.58	0.36	-1.01	-0.26	0.44
Co	0.06	0.01	-0.80	-1.47	0.29	-0.19	-0.08	0.96	0.25
CO32-	-	-	-	-	-	-	-	-	-
Cr	0.01	1.47	1.68	0.54	-0.57	-0.90	-0.07	0.83	0.33
Cu	0.03	0.85	2.82	1.75	1.55	1.48	0.33	1.12	0.53
Fe	0.03	1.00	1.19	1.04	0.52	0.89	2.16	2.51	0.49
B	0.04	0.08	0.17	0.45	0.88	-0.59	-2.27	-2.25	0.43
Si	-0.92	-0.15	0.13	0.12	0.10	0.44	1.00	0.68	0.20
K	0.22	0.01	0.08	0.08	0.11	0.64	0.96	0.60	0.17
Li	0.04	0.10	0.26	0.45	0.74	1.06	1.80	1.10	0.32
Mg	0.04	0.14	0.30	-0.24	0.17	0.70	-0.15	-0.69	0.14
Mn	0.04	0.19	0.34	-0.91	0.73	1.75	0.15	-1.36	0.32
Mo	1.69	1.01	1.68	-0.01	0.04	0.20	0.34	0.06	0.33
Na	0.39	0.41	-0.83	0.63	0.77	0.87	1.04	-1.49	0.31
Ni	0.04	0.13	-0.29	-0.76	0.38	-0.94	-0.56	0.84	0.21
Pb	0.04	1.01	0.04	-1.62	-0.86	-0.37	0.79	2.78	0.45
PO4	-	-	-	-	-	-	-	-	-
Sb	0.04	-0.38	0.24	1.32	1.32	0.69	-0.77	0.26	0.27
Se	0.04	0.08	0.09	0.77	1.44	1.48	-0.09	1.25	0.32
Sn	0.01	-0.36	-0.07	-0.38	-0.07	0.76	2.48	1.41	0.38
SO4	-	-	-	-	-	-	-	-	-
Sr	0.04	0.07	0.14	0.39	0.78	0.83	1.44	0.66	0.25
V	0.04	1.00	-0.17	1.26	1.52	1.35	-0.01	0.79	0.34
Zn	0.04	0.08	0.87	-0.21	-0.67	0.65	-1.36	1.01	0.27
Avg Deviation	0.08	0.12	0.20	0.19	0.17	0.18	0.22	0.24	0.31