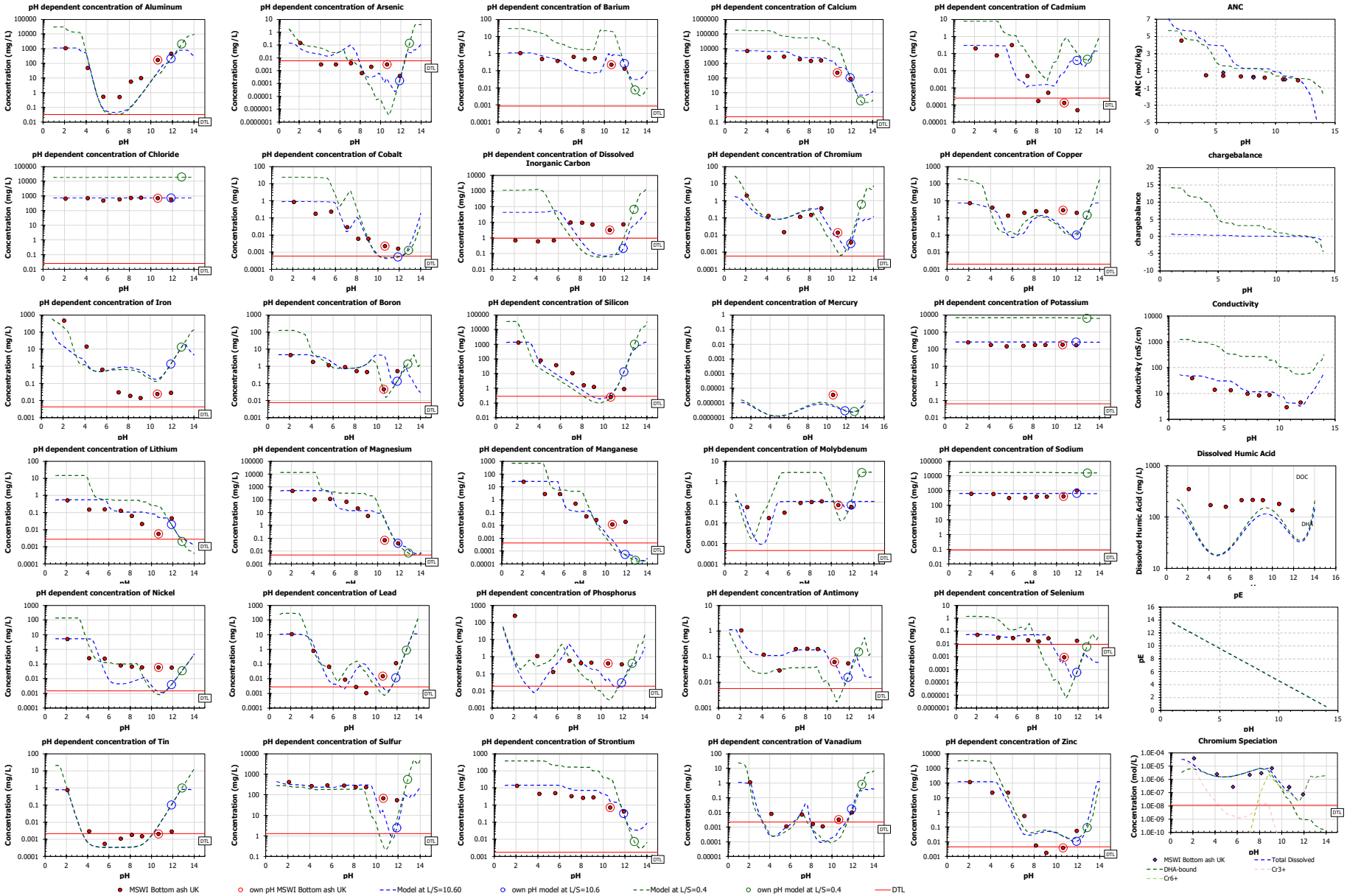
MSWI Bottom ash UK

COMPARISON pH DEPENDENCE TEST DATA WITH MODEL



Object pH Dependent Leaching Test Model
Name MSWI Bottom ash UK

pH Dependent Leaching Test Scenario

Lab Test

Extra L/S Simulation

Lab Test

Model Parameters

Entity	Unit	Default
c0		-4.433
c1		0.7928
c2		-0.5870
c3		0.1258
c4		-0.01053
c5		0.0003037
Clay	mg/kg	3000
Hydrous Ferric Oxide	mg/kg	650.0
L/S	L/kg	10.60
pE		3.950
pH		10.65
Solid Humic Acid	mg/kg	5000
Simulated Low L/S	L/kg	0.4000

Available Content

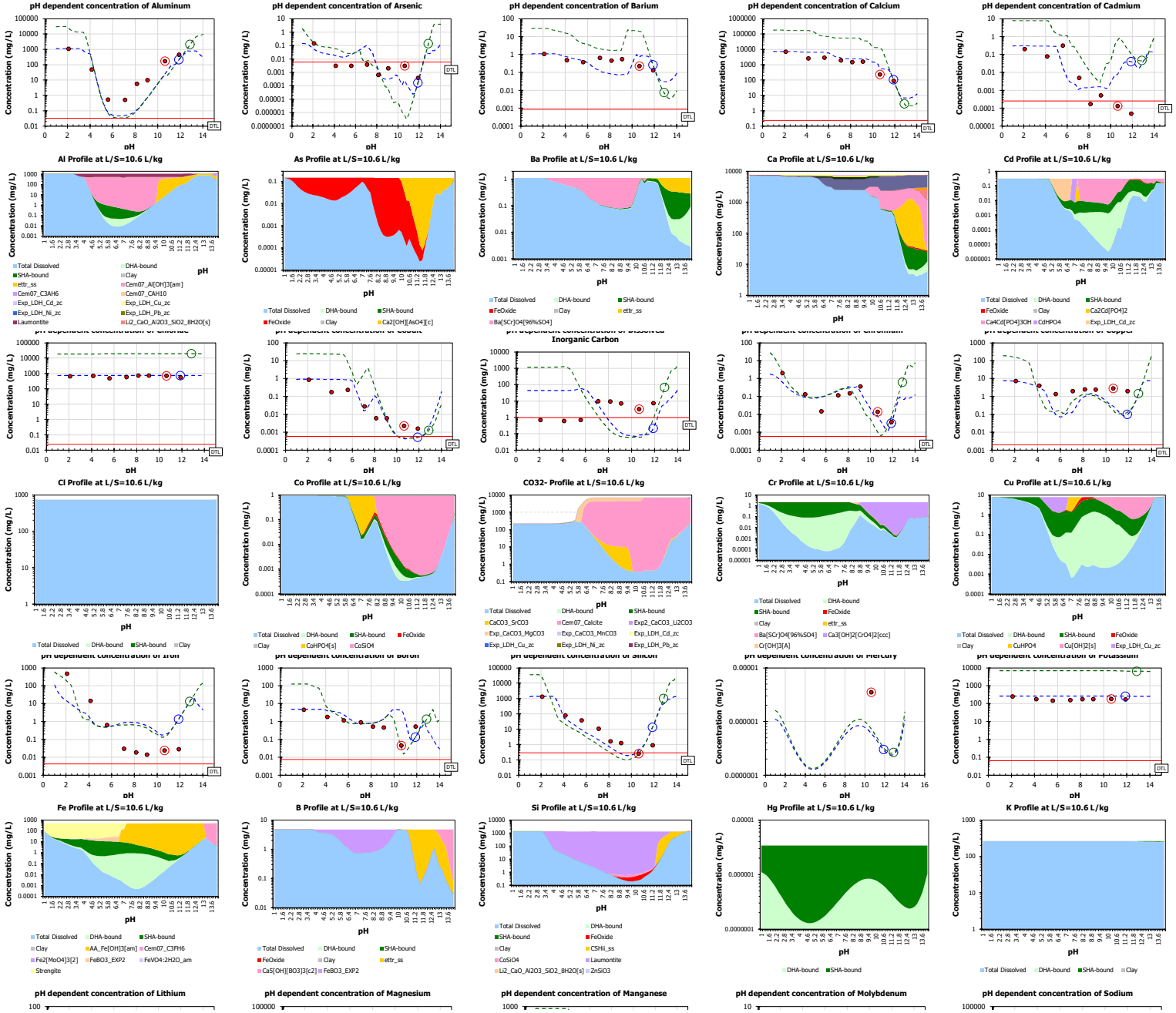
Entity	mg/kg	Entity	mg/kg	Entity	mg/kg	Entity	mg/kg
Al	1.226E+04	B	50.35	Sb	11.87		
As	1.583	Si	1.449E+04	Se	0.5608		
Ba	11.75	Hg	3.620E-05	Sn	8.468		
Ca	7.812E+04	K	2790	SO4	1.404E+04		
Cd	3.222	Li	5.821	Sr	150.9		
Cl	7754	Mg	5341	V	12.50		
Co	9.671	Mn	278.9	Zn	1323		
CO32-	7.200E+04	Mo	1.163				
Cr	22.79	Na	6812				
Cu	82.04	Ni	56.23				
F	1.900E-09	Pb	119.8				
Fe	5207	PO4	8527				

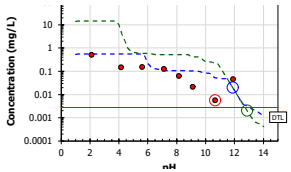
Solid Solutions

Name	End Member	Log(K)	Reaction
CSHii_ss	Cem07_Jenn_ss	-7.799	Cem07_Jenn_ss + 1.33333 H+ -> 1 CSHii_ss + 1.66667 Ca+2 + 1.76667 H2O + 1 H2SiO4-2
	Cem07_Tob_II_ss	10.36	Cem07_Tob_II_ss -> 1 CSHii_ss + 0.83333 Ca+2 + 0.33333 H+ + 0.16667 H2O + 1 H2SiO4-2
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

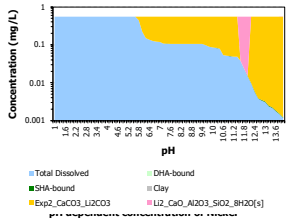
Minerals

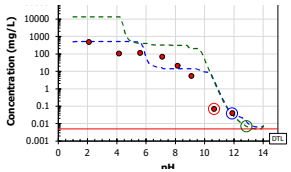
Name	Log(K)	Reaction
AA_Fe[OH]3[am]	16.60	AA_Fe[OH]3[am] + 1 H2O -> 1 Fe[OH]4- + 1 H+
alpha-TCP	25.50	alpha-TCP -> 3 Ca+2 + 2 PO4-3
Ba[SCr]O4[96%SO4]	9.790	Ba[SCr]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2
Ca2[OH][AsO4][c]	4.000	Ca2[OH][AsO4][c] + 1 H+ -> 1 AsO4-3 + 2 Ca+2 + 1 H2O
Ca2Cd[PO4]2	32.95	Ca2Cd[PO4]2 -> 2 Ca+2 + 1 Cd+2 + 2 PO4-3
Ca3[OH]2[CrO4]2[ccc]	1.000	Ca3[OH]2[CrO4]2[ccc] + 2 H+ -> 3 Ca+2 + 2 CrO4-2 + 2 H2O
Ca4Cd[PO4]3OH	39.23	Ca4Cd[PO4]3OH + 1 H+ -> 4 Ca+2 + 1 Cd+2 + 1 H2O + 3 PO4-3
Ca5[OH][BO3]3[c2]	-53.00	Ca5[OH][BO3]3[c2] + 7 H+ -> 5 Ca+2 + 3 H2BO3- + 1 H2O
CaCO3_SrCO3	19.85	CaCO3_SrCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Sr+2
CaSb[OH]6[s]2	19.41	CaSb[OH]6[s]2 -> 1 Ca+2 + 2 Sb[OH]6-
Cd[OH]2[C]	-13.65	Cd[OH]2[C] + 2 H+ -> 1 Cd+2 + 2 H2O
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_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_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
CoHPO4[s]	24.48	CoHPO4[s] -> 1 Co+2 + 1 H+ + 1 PO4-3
CoSiO4	6.289	CoSiO4 + 2 H+ -> 2 Co+2 + 1 H2SiO4-2
Cr[OH]3[A]	68.13	Cr[OH]3[A] + 1 H2O -> 1 CrO4-2 + 5 H+ + 3 e-
Cu[OH]2[s]	-8.640	Cu[OH]2[s] + 2 H+ -> 1 Cu+2 + 2 H2O
CuHPO4	26.00	CuHPO4 -> 1 Cu+2 + 1 H+ + 1 PO4-3
Exp_CaCO3_MgCO3	19.00	Exp_CaCO3_MgCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Mg+2
Exp_CaCO3_MnCO3	21.48	Exp_CaCO3_MnCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Mn+2
Exp_LDH_Cd_zc	60.06	Exp_LDH_Cd_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 3 Cd+2 + 1 H+
Exp_LDH_Cu_zc	58.21	Exp_LDH_Cu_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 3 Cu+2 + 1 H+
Exp_LDH_Ni_zc	57.91	Exp_LDH_Ni_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 1 H+ + 3 Ni+2
Exp_LDH_Pb_zc	63.00	Exp_LDH_Pb_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 1 H+ + 3 Pb+2
Exp2_Ca[OH]Sb[OH]6	1.000	Exp2_Ca[OH]Sb[OH]6 + 1 H+ -> 1 Ca+2 + 1 H2O + 1 Sb[OH]6-
Exp2_Ca2[OH]2[SeO4]	-8.000	Exp2_Ca2[OH]2[SeO4] + 2 H+ -> 2 Ca+2 + 2 H2O + 1 SeO4-2
Exp2_CaCO3_Li2CO3	25.14	Exp2_CaCO3_Li2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 Li+
Fe2[MoO4]3[2]	86.35	Fe2[MoO4]3[2] + 8 H2O -> 2 Fe[OH]4- + 8 H+ + 3 MoO4-2
FeBO3_EXP2	30.00	FeBO3_EXP2 + 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+
Laumontite	118.0	Laumontite + 8 H2O -> 2 Al[OH]4- + 1 Ca+2 + 8 H+ + 4 H2SiO4-2
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+
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
Pb[OH]2[C]	-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
PbHPO4	28.00	PbHPO4 -> 1 H+ + 1 PO4-3 + 1 Pb+2
Sn[OH]2[s]	1.447	Sn[OH]2[s] + 2 H+ -> 2 H2O + 1 Sn+2
Strengite	48.00	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
ZnHPO4	24.48	ZnHPO4 -> 1 H+ + 1 PO4-3 + 1 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=10.6 L/kg
As Profile at L/S=10.6 L/kg
Ba Profile at L/S=10.6 L/kg
Ca Profile at L/S=10.6 L/kg
Cd Profile at L/S=10.6 L/kg
Inorganic Carbon
Cl Profile at L/S=10.6 L/kg
Co Profile at L/S=10.6 L/kg
CO32- Profile at L/S=10.6 L/kg
Cr Profile at L/S=10.6 L/kg
Cu Profile at L/S=10.6 L/kg
Fe Profile at L/S=10.6 L/kg
B Profile at L/S=10.6 L/kg
Si Profile at L/S=10.6 L/kg
Hg Profile at L/S=10.6 L/kg
K Profile at L/S=10.6 L/kg
pH dependent concentration of Lithium
pH dependent concentration of Magnesium
pH dependent concentration of Manganese
pH dependent concentration of Molybdenum
pH dependent concentration of Sodium
Concentration (mg/L)
pH
Total Dissolved
DHA-bound
SHA-bound
Clay
FeOxide
CaCO3_SrCO3
Cem07_Calcite
Exp2_CaCO3_Li2CO3
Exp_CaCO3_MgCO3
Exp_CaCO3_MnCO3
Exp_LDH_Cd_zc
Exp_LDH_Cu_zc
Exp_LDH_Ni_zc
Exp_LDH_Pb_zc
CoHPO4[s]
CoSiO4
Ca2Cd[PO4]2
Ca4Cd[PO4]3OH
CdHPO4
Cu[OH]2[s]
CuHPO4
Ettr_ss
Cem07_Al[OH]3[am]
Cem07_C3AH6
Cem07_CAH10
Exp_LDH_Ni_zc
Laumontite
Li2_CaO_Al2O3_SiO2_8H2O[s]
Ba[SCr]O4[96%SO4]
Ca2[OH][AsO4][c]
Ca3[OH]2[CrO4]2[ccc]
Cr[OH]3[A]
Fe2[MoO4]3[2]
FeBO3_EXP2
FeVO4:2H2O_am
Strengite
Ca5[OH][BO3]3[c2]
CSHii_ss
ZnSiO3

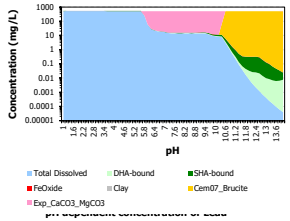


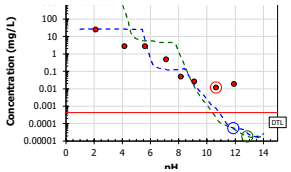
Li Profile at L/S=10.6 L/kg



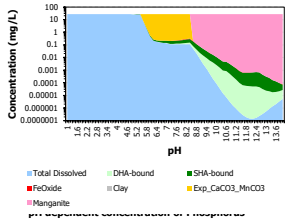


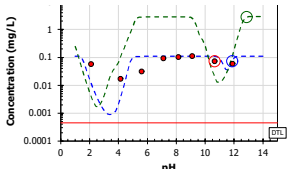
Mg Profile at L/S=10.6 L/kg



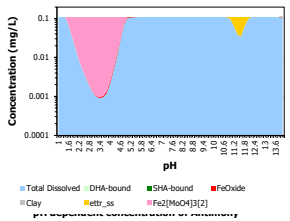


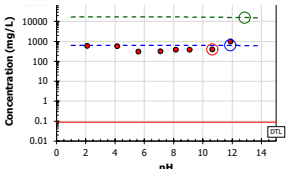
Mn Profile at L/S=10.6 L/kg



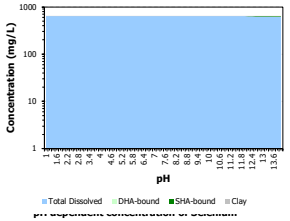


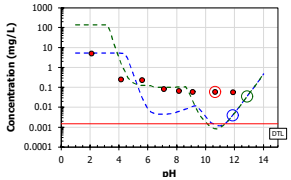
Mo Profile at L/S=10.6 L/kg



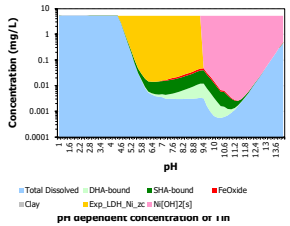


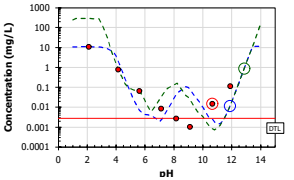
Na Profile at L/S=10.6 L/kg



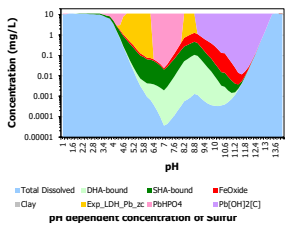


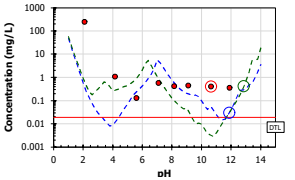
Ni Profile at L/S=10.6 L/kg



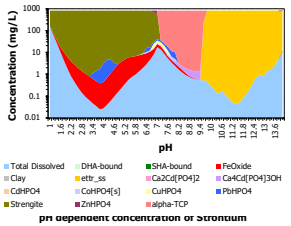


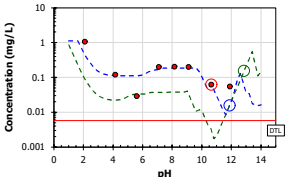
Pb Profile at L/S=10.6 L/kg



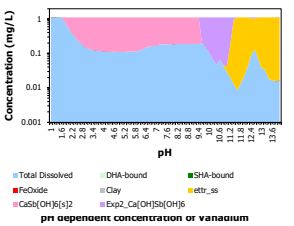


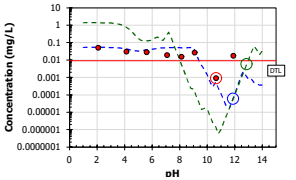
PO4 Profile at L/S=10.6 L/kg



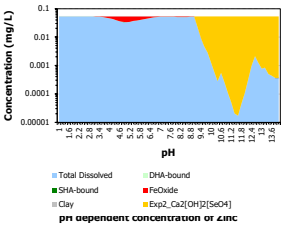


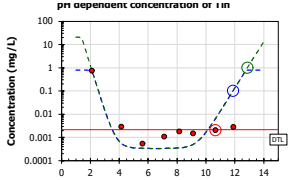
Sb Profile at L/S=10.6 L/kg



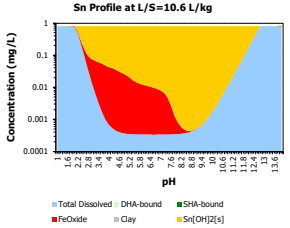


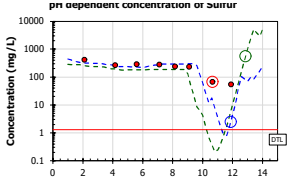
Se Profile at L/S=10.6 L/kg



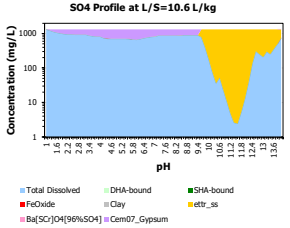


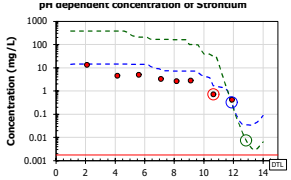
Sn Profile at L/S=10.6 L/kg



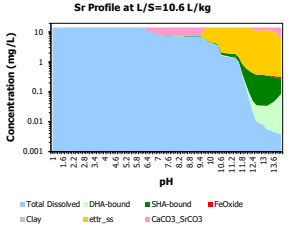


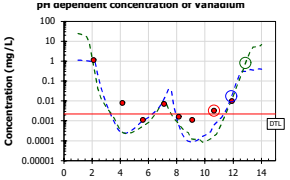
SO4 Profile at L/S=10.6 L/kg



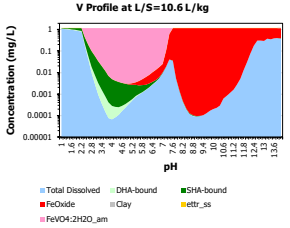


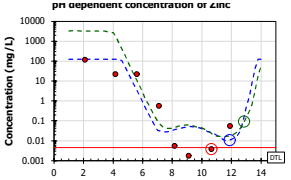
Sr Profile at L/S=10.6 L/kg



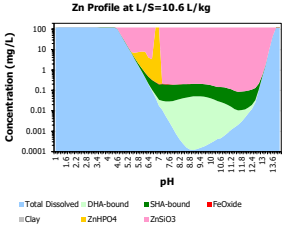


V Profile at L/S=10.6 L/kg





Zn Profile at L/S=10.6 L/kg



Model Comparison: residuals - Concentration

Name **MSWI Bottom ash UK**

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	*2.10*	*4.15*	*5.60*	*7.10*	*8.15*	*9.10*	*10.7*	*11.9*	*Deviation*
Al	0.03	0.58	-0.84	-1.00	-1.69	-1.10	-0.80	-0.29	0.33
As	-0.42	0.77	0.86	1.37	0.39	-0.78	-1.12	-0.28	0.29
Ba	0.03	0.19	0.08	-0.72	-0.74	-0.86	0.50	0.25	0.18
Br	-	-	-	-	-	-	-	-	-
Ca	0.02	0.42	0.36	0.17	0.22	0.19	0.40	0.03	0.10
Cd	0.19	0.58	-1.23	-0.61	0.94	0.47	1.81	2.89	0.48
Cl	0.05	0.03	0.18	0.11	0.00	0.00	0.03	0.12	0.03
Co	0.03	0.71	0.58	-0.23	1.17	-0.15	-0.71	-0.47	0.22
CO32-	-	-	-	-	-	-	-	-	-
Cr	-0.51	-0.17	0.81	0.26	0.36	-0.30	-0.25	-0.01	0.14
Cu	-0.01	-0.10	-1.16	-1.12	-0.38	-0.28	-1.01	-1.28	0.29
F	-	-	-	-	-	-	-	-	-
Fe	-1.53	-1.02	-0.11	1.45	1.65	1.62	0.89	1.72	0.48
B	0.03	0.35	0.31	-0.07	0.21	0.50	1.96	-0.55	0.27
Si	0.03	-0.21	-0.62	-0.72	-0.41	-0.70	0.25	1.23	0.22
Hg	-	-	-	-	-	-	-0.77	-	0.77
K	0.03	0.18	0.26	0.23	0.18	0.18	0.16	0.19	0.07
Li	0.03	0.57	0.56	-0.05	0.22	0.69	0.97	-0.40	0.19
Mg	0.03	0.69	0.64	-0.64	-0.17	0.42	1.61	-0.04	0.25
Mn	0.03	0.98	0.40	-0.57	0.44	-0.16	-1.21	-2.54	0.39
Mo	-0.70	-0.64	0.54	0.08	0.04	0.00	0.17	0.12	0.14
Na	0.03	0.05	0.32	0.30	0.23	0.22	0.21	-0.19	0.08
Ni	0.02	1.32	-0.88	-1.25	-1.01	-0.72	-1.61	-1.13	0.39
NO3	-	-	-	-	-	-	-	-	-
Pb	0.01	0.39	-0.94	-0.56	1.21	1.87	-0.76	-0.93	0.35
PO4	-	-	-	-	-	-	-	-	-
Sb	-0.37	-0.03	0.58	-0.05	-0.04	-0.03	-0.02	-0.51	0.11
Se	0.03	0.15	0.13	0.44	0.51	0.12	-0.31	-2.41	0.32
Sn	-0.09	-0.72	-0.20	-0.51	-0.71	-0.47	0.50	1.59	0.26
SO4	-	-	-	-	-	-	-	-	-
Sr	0.03	0.50	0.45	0.39	0.44	0.41	0.38	-0.16	0.13
Th	-	-	-	-	-	-	-	-	-
U	-	-	-	-	-	-	-	-	-
V	-0.10	-1.50	-0.06	0.26	-0.44	-1.09	-0.68	0.30	0.26
Zn	0.03	0.75	-0.82	-1.23	0.82	1.47	0.83	-0.70	0.32
Avg Deviati	0.07	0.13	0.12	0.14	0.14	0.15	0.18	0.22	0.26

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