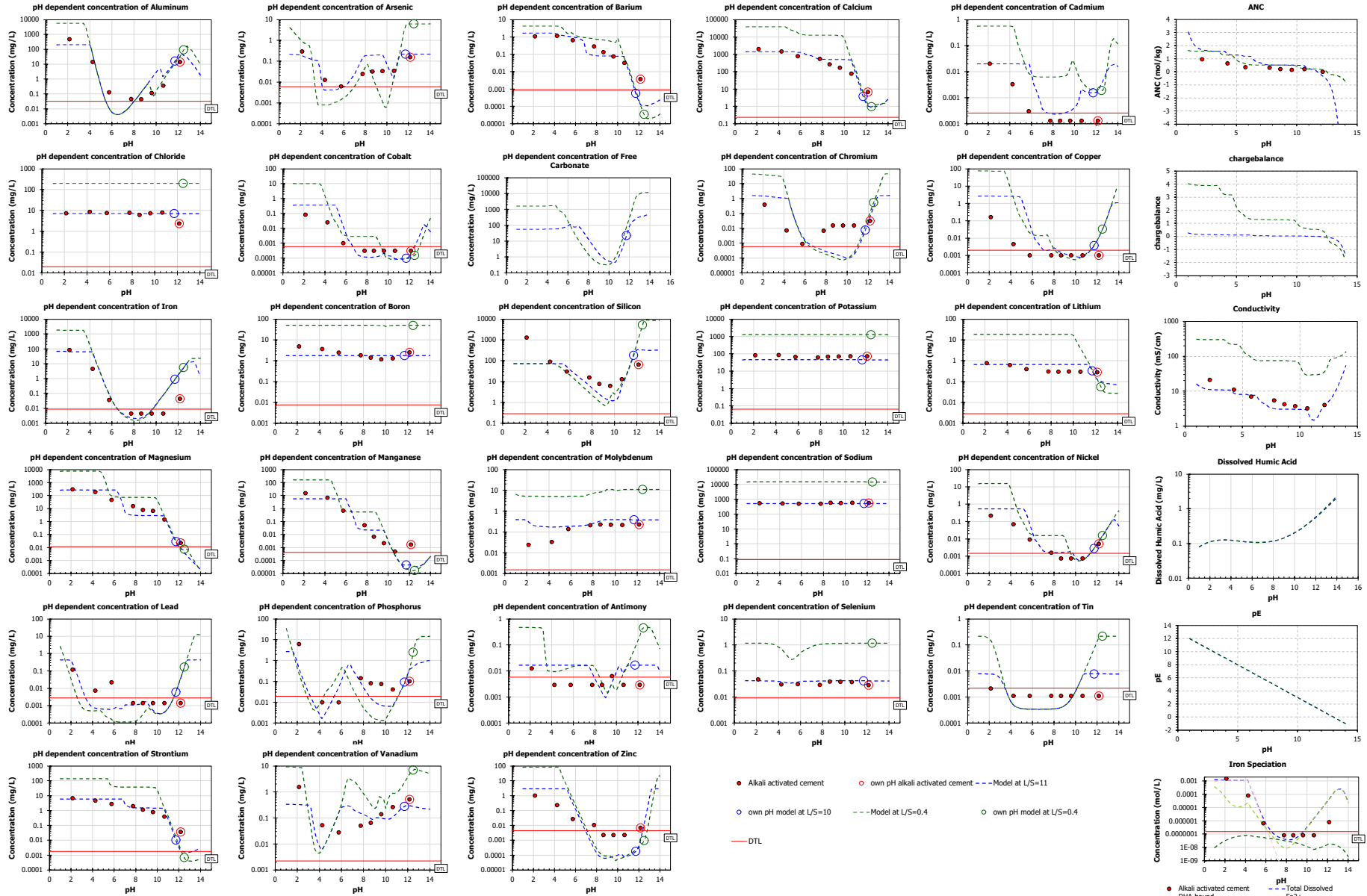


Alkali activated cement

COMPARISON pH DEPENDENCE WITH MODEL



Object Name pH Dependent Leaching Test Model
Alkali activated cement

pH Dependent Leaching Test Scenario



Lab Test

Extra L/S Simulation

Lab Test

Model Parameters

Entity	Unit	Default	Entity	mg/kg	Entity	mg/kg	Entity	mg/kg
c0		-7.684	Al	2300	B	20.04	PO4	105.1
c1		0.3742	As	2.509	Si	4600	Sb	0.1892
c2		-0.09601	Ba	19.06	Hg	2.006E-07	Se	0.4700
c3		0.008996	Br	1.080	K	510.0	Sn	0.08675
c4		-0.0002446	Ca	1.600E+04	Li	7.500	SO4	1720
c5		0	Cd	0.2262	Mg	2970	Sr	66.65
Clay	mg/kg	1000	Cl	80.16	Mn	63.23	Th	2.320E-07
Hydrous Ferric Oxide	mg/kg	90.00	Co	4.058	Mo	4.383	U	2.380E-07
L/S	L/kg	11.28	CO32-	2.020E+04	Na	5800	V	3.805
pE		0.2000	Cr	18.30	Ni	6.133	Zn	33.14
pH		12.80	Cu	30.35	NO3	6.200E-08		
Solid Humic Acid	mg/kg	200.0	Fe	780.0	Pb	4.936		
Simulated Low L/S	L/kg	0.4000						

Solid Solutions

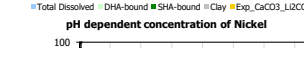
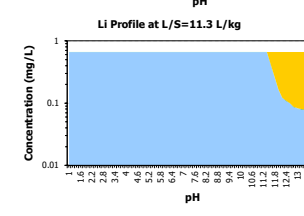
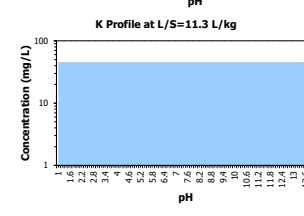
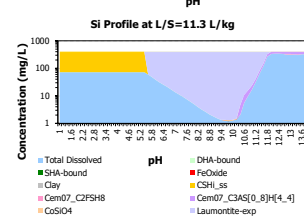
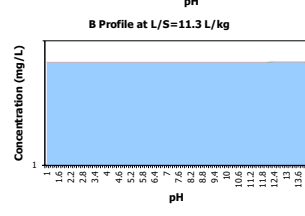
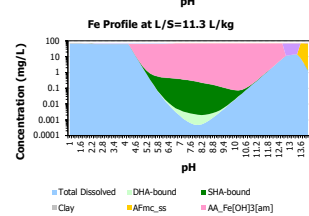
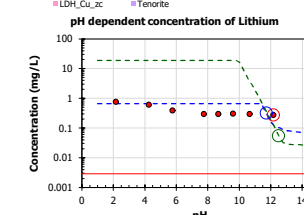
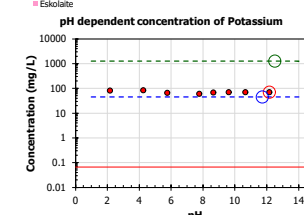
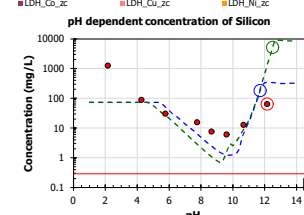
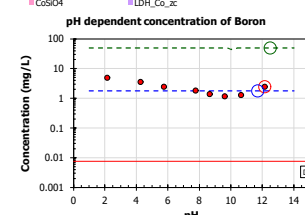
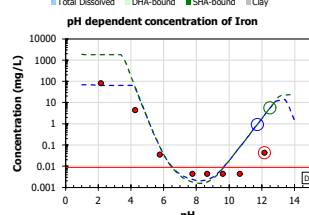
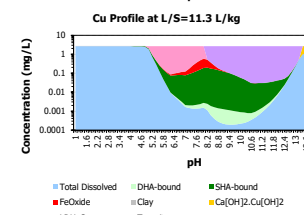
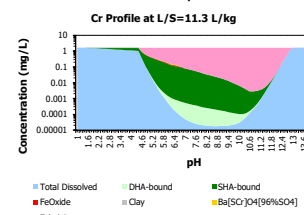
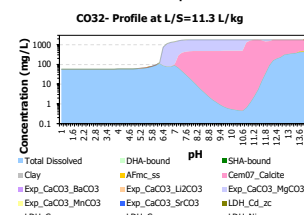
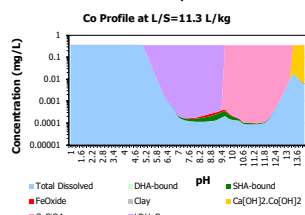
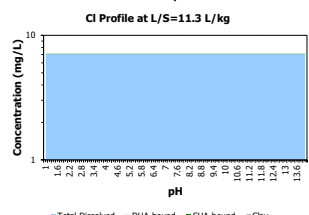
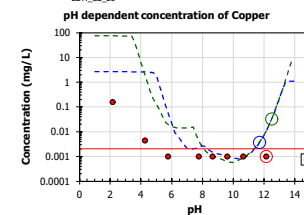
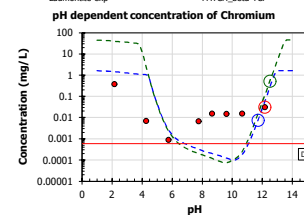
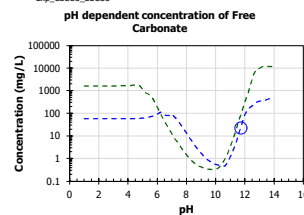
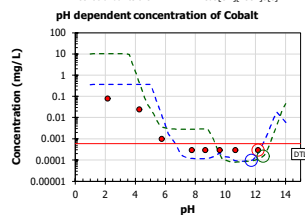
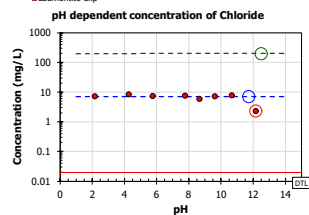
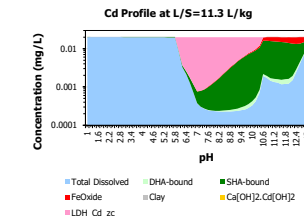
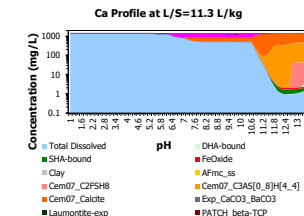
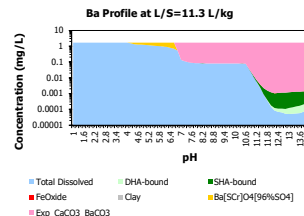
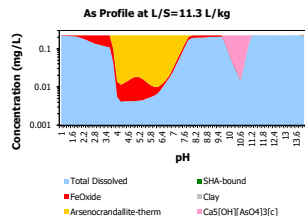
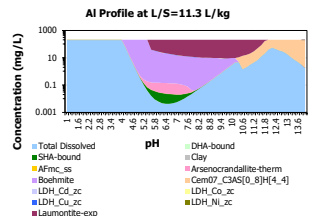
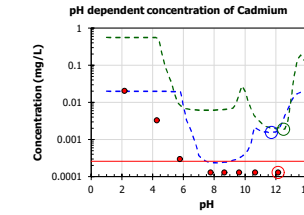
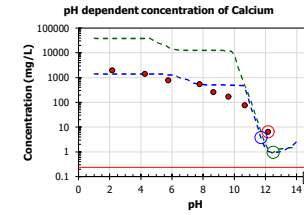
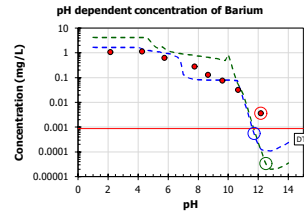
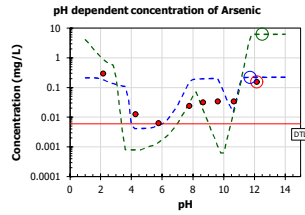
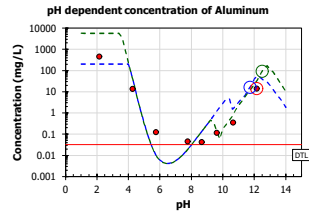
Name	End Member	Log(K)	Reaction
AFmc_ss	Cem07_C4Ach11_ss	-24.50	Cem07_C4Ach11_ss + 4 H+ -> 1 AFmc_ss + 2 Al[OH]4- + 1 CO3-2 + 4 Ca+2 + 9 H2O
	Cem07_C4Fch12_ss	-20.47	Cem07_C4Fch12_ss + 4 H+ -> 1 AFmc_ss + 1 CO3-2 + 4 Ca+2 + 2 Fe[OH]4- + 10 H2O

Minerals

Name	Log(K)	Reaction	Name	Log(K)	Reaction
AA_Fe[OH]3[am]	16.60	AA_Fe[OH]3[am] + 1 H2O -> 1 Fe[OH]4- + 1 H+	Exp_CaCO3_Li2CO3	21.30	Exp_CaCO3_Li2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 Li+
Antimocrandallite-e	63.00	Antimocrandallite-exp + 8 H2O -> 3 Al[OH]4- + 1 Ca+2 + 3 H+ + 2 Sb[OH]6-	Exp_CaCO3_MgCO3	19.00	Exp_CaCO3_MgCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Mg+2
Arsenocrandallite-tr	95.56	Arsenocrandallite-therm + 6 H2O -> 3 Al[OH]4- + 2 AsO4-3 + 1 Ca+2 + 7 H+	Exp_CaCO3_MnCO3	21.48	Exp_CaCO3_MnCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Mn+2
Ba[Scr]O4[96%SO4]	9.790	Ba[Scr]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2	Exp_CaCO3_SrCO3	19.85	Exp_CaCO3_SrCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Sr+2
BaSrSO4[50%Ba]	8.221	BaSrSO4[50%Ba] -> 0.5 Ba+2 + 1 SO4-2 + 0.5 Sr+2	Fe_Vanadate	19.18	Fe_Vanadate + 1 H2O -> 0.5 Fe[OH]4- + 1 VO2+ + 0.5 e-
Boehmite	14.07	Boehmite + 2 H2O -> 1 Al[OH]4- + 1 H+	Laumontite-exp	116.0	Laumontite-exp + 8 H2O -> 2 Al[OH]4- + 1 Ca+2 + 8 H+ + 4 H2SiO4-2
Ca[OH]2.Cd[OH]2	-34.00	Ca[OH]2.Cd[OH]2 + 4 H+ -> 1 Ca+2 + 1 Cd+2 + 4 H2O	LDH_Cd_zc	60.06	LDH_Cd_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 3 Cd+2 + 1 H+
Ca[OH]2.Co[OH]2	-32.40	Ca[OH]2.Co[OH]2 + 4 H+ -> 1 Ca+2 + 1 Co+2 + 4 H2O	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.Ni[OH]2	-32.00	Ca[OH]2.Ni[OH]2 + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Ni+2	LDH_Ni_zc	57.91	LDH_Ni_zc + 1 H2O -> 1 Al[OH]4- + 3 CO3-2 + 1 H+ + 3 Ni+2
Ca[OH]2.Zn[OH]2	-30.52	Ca[OH]2.Zn[OH]2 + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Zn+2	Manganite	-25.27	Manganite + 3 H+ + 1 e- -> 2 H2O + 1 Mn+2
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-	Ni[OH]2[s]	-10.80	Ni[OH]2[s] + 2 H+ -> 2 H2O + 1 Ni+2
Ca5[OH][AsO4]3[c]	26.13	Ca5[OH][AsO4]3[c] + 1 H+ -> 3 AsO4-3 + 5 Ca+2 + 1 H2O	PATCH_beta-TCP	28.93	PATCH_beta-TCP -> 3 Ca+2 + 2 PO4-3
Cd[OH]2[C]	-13.65	Cd[OH]2[C] + 2 H+ -> 1 Cd+2 + 2 H2O	Pb[OH]2[C]	-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
Cem07_Brucite	-16.83	Cem07_Brucite + 2 H+ -> 2 H2O + 1 Mg+2	Pb2V2O7	0.9500	Pb2V2O7 + 3 H+ -> 1.5 H2O + 1 Pb+2 + 1 VO2+
Cem07_C2FSH8	21.41	Cem07_C2FSH8 -> 2 Ca+2 + 2 Fe[OH]4- + 3 H2O + 1 H2SiO4-2	Pb3[VO4]2	-3.070	Pb3[VO4]2 + 4 H+ -> 2 H2O + 1.5 Pb+2 + 1 VO2+
Cem07_C3AS[O_8]H	-5.555	Cem07_C3AS[O_8]H[4_4] + 2.4 H+ -> 2 Al[OH]4- + 3 Ca+2 + 0.8 H2O + 0.8 H2SiO4-2	PbMoO4[c]	15.80	PbMoO4[c] -> 1 MoO4-2 + 1 Pb+2
Cem07_Calcite	8.485	Cem07_Calcite -> 1 CO3-2 + 1 Ca+2	PbOH[Sb[OH]6]_exp1	12.00	PbOH[Sb[OH]6]_exp1 + 1 H+ -> 1 H2O + 1 Pb+2 + 1 Sb[OH]6-
Cem07_Gypsum	4.583	Cem07_Gypsum -> 1 Ca+2 + 2 H2O + 1 SO4-2	Sn[OH]2[s]	1.447	Sn[OH]2[s] + 2 H+ -> 2 H2O + 1 Sn+2
CoSiO4	6.289	CoSiO4 + 2 H+ -> 2 Co+2 + 1 H2SiO4-2	Strengite	48.00	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
Eskolaite	139.5	Eskolaite + 5 H2O -> 2 CrO4-2 + 10 H+ + 6 e-	Tenorite	-7.620	Tenorite + 2 H+ -> 1 Cu+2 + 1 H2O
Exp_Antimocrandall	63.00	Exp_Antimocrandallite + 8 H2O -> 3 Al[OH]4- + 1 Ca+2 + 3 H+ + 2 Sb[OH]6-	ZnSiO3_MQ	18.69	ZnSiO3_MQ + 1 H2O -> 1 H2SiO4-2 + 1 Zn+2
Exp_CaCO3_BaCO3	21.30	Exp_CaCO3_BaCO3 -> 1 Ba+2 + 2 CO3-2 + 1 Ca+2			

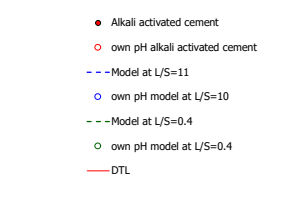
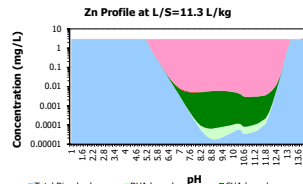
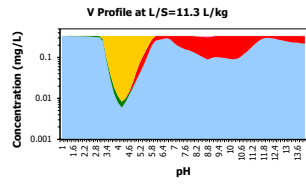
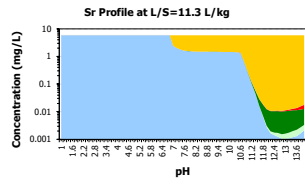
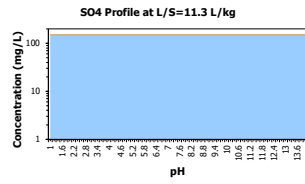
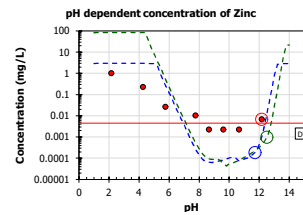
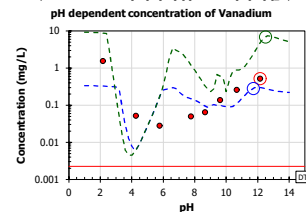
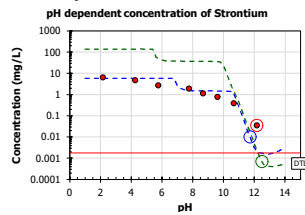
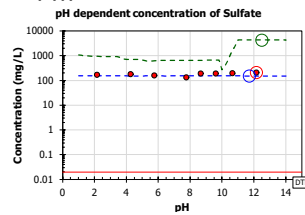
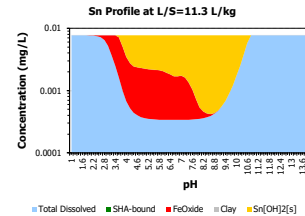
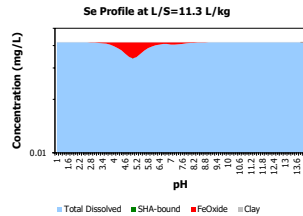
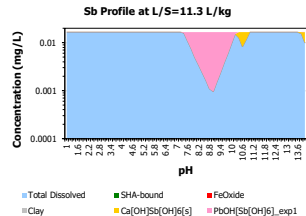
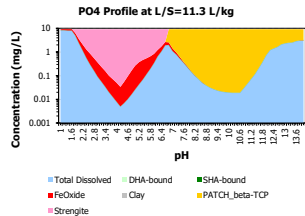
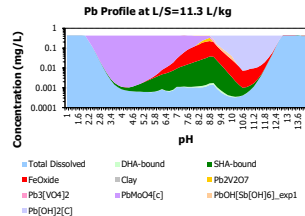
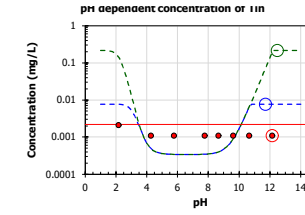
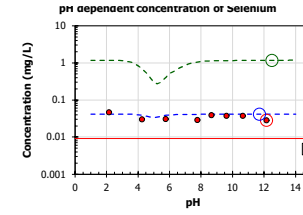
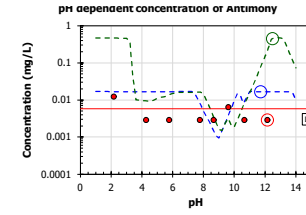
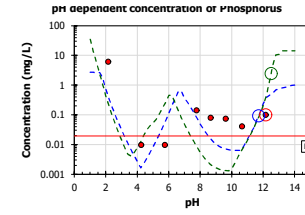
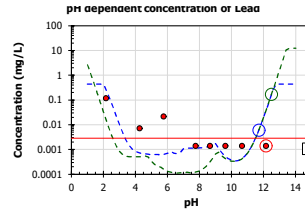
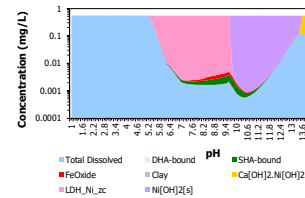
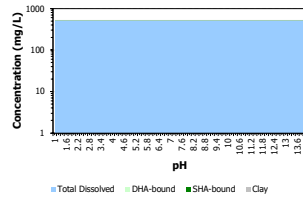
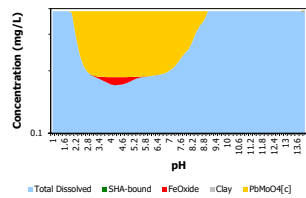
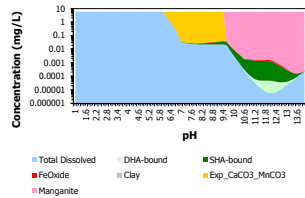
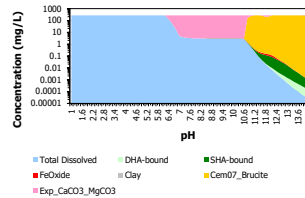
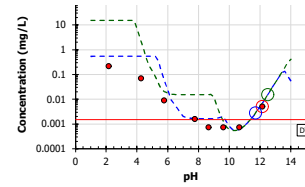
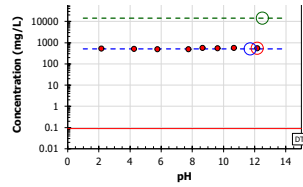
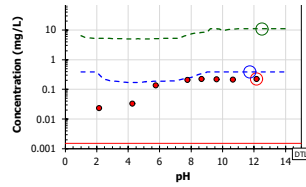
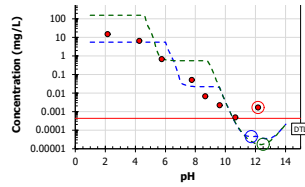
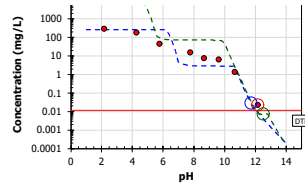
ALKALI ACTIVATED CEMENT

COMPARISON AND PARTITIONING



ALKALI ACTIVATED CEMENT

COMPARISON AND PARTITIONING



Model Comparison: residuals - Concentration

Name Alkali activated cement

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	2.15	4.25	5.75	7.75	8.65	9.60	10.7	12.2	Deviation
Al	-0.36	0.50	-1.09	-0.38	0.49	1.00	0.66	0.57	0.24
As	-0.21	-0.48	-0.08	0.78	0.78	0.78	-0.27	0.15	0.19
Ba	0.20	0.10	0.19	-0.52	-0.21	0.02	0.28	-1.45	0.20
Br	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.98	0.35
Ca	-0.14	-0.01	0.22	0.00	0.29	0.47	0.70	-0.78	0.15
Cd	-0.01	0.78	1.81	0.27	0.27	0.38	1.21	1.15	0.33
Cl	-0.01	-0.07	-0.02	-0.03	0.07	-0.01	-0.05	0.49	0.06
Co	0.65	1.16	1.12	-0.40	-0.41	-0.15	-0.51	-0.15	0.24
Cr	0.59	2.17	0.48	-1.32	-1.88	-2.09	-1.92	0.26	0.54
Cu	1.22	2.76	1.78	0.36	0.17	0.01	-0.09	1.04	0.46
Fe	-0.10	1.06	0.37	-0.27	-0.28	0.27	1.26	1.76	0.31
B	-0.44	-0.31	-0.14	-0.01	0.10	0.18	0.14	-0.15	0.08
Si	-1.25	-0.10	0.23	-0.38	-0.49	-0.69	-0.31	0.72	0.22
K	-0.26	-0.27	-0.17	-0.14	-0.18	-0.19	-0.20	-0.20	0.07
Li	-0.07	0.03	0.22	0.34	0.35	0.34	0.35	-0.33	0.10
Mg	-0.05	0.16	0.77	-0.71	-0.43	-0.36	0.21	-0.38	0.16
Mn	-0.42	-0.08	0.92	-0.34	0.51	0.94	-0.31	-1.58	0.28
Mo	1.12	0.71	0.14	0.06	0.17	0.25	0.26	0.24	0.18
Na	-0.02	-0.01	0.01	0.01	-0.05	-0.03	-0.04	-0.04	0.01
Ni	0.40	0.89	0.87	0.02	0.34	0.44	-0.08	0.14	0.18
Pb	0.35	-1.00	-1.54	-0.10	0.01	-0.43	-0.52	1.42	0.30
PO4	-	-	-	-	-	-	-	-	-
Sb	0.13	0.76	0.76	0.45	-0.29	-0.23	0.49	0.76	0.19
Se	-0.05	0.10	0.10	0.15	0.02	0.04	0.05	0.17	0.03
Sn	0.56	-0.34	-0.51	-0.50	-0.44	-0.09	0.76	0.85	0.19
SO4	-0.05	-0.07	-0.03	0.06	-0.10	-0.10	-0.11	-0.14	0.03
Sr	-0.05	0.10	0.34	-0.09	0.12	0.28	0.47	-1.22	0.17
V	-0.68	-0.91	0.77	0.48	0.17	-0.14	-0.37	-0.24	0.19
Zn	0.46	1.10	1.01	-1.58	-1.56	-1.43	-1.47	-0.82	0.44
Avg Deviat	0.10	0.17	0.15	0.10	0.11	0.12	0.13	0.15	0.21

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