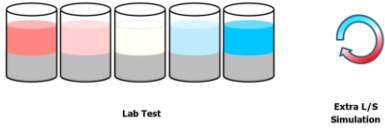


Object Name
pH Dependent Leaching Test Model
Alkaline Coal fly ash NL

pH Dependent Leaching Test Scenario



Lab Test

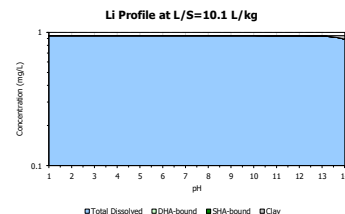
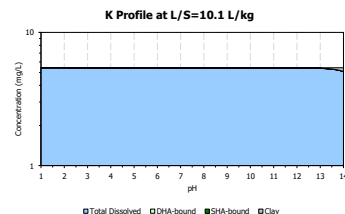
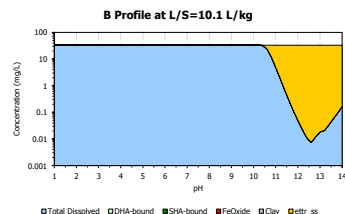
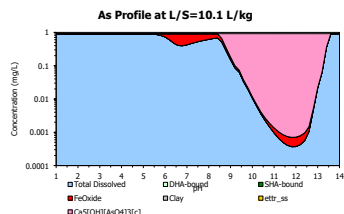
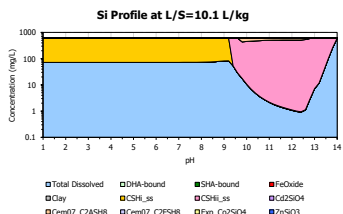
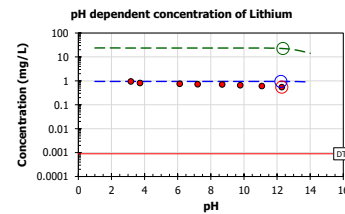
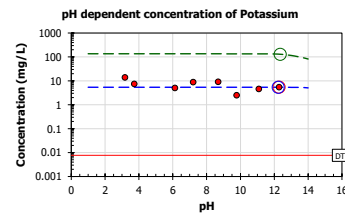
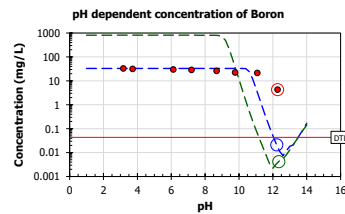
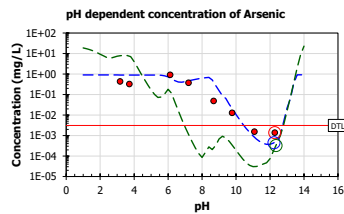
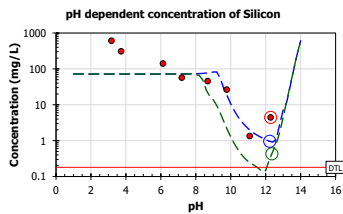
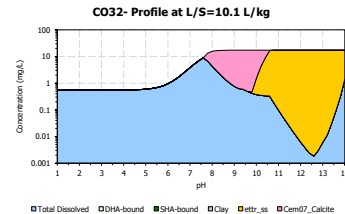
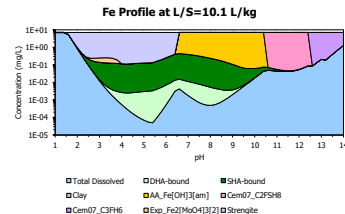
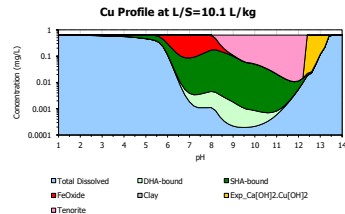
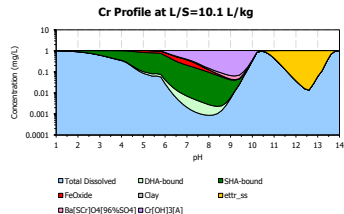
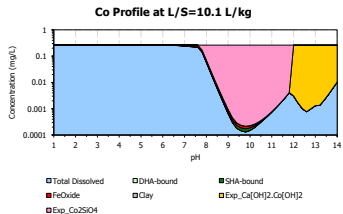
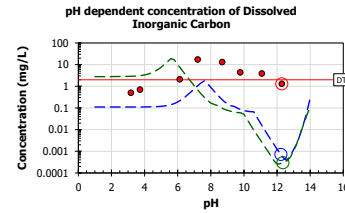
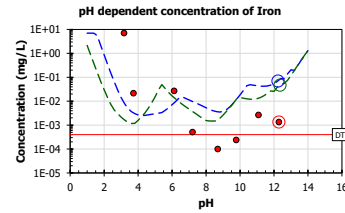
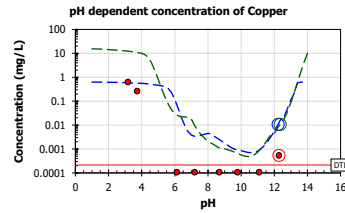
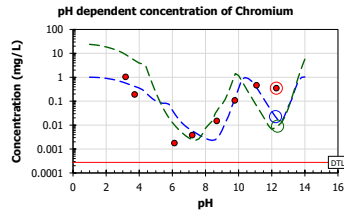
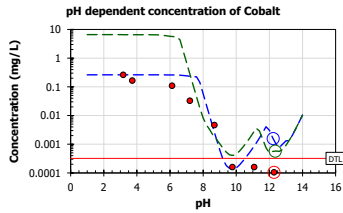
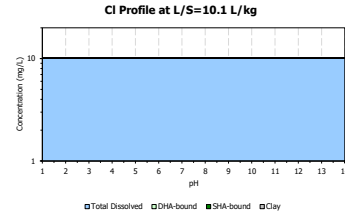
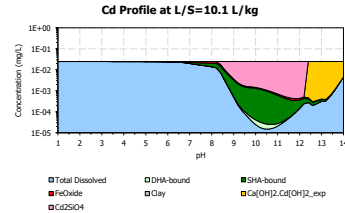
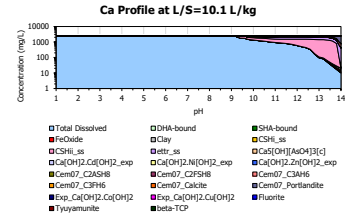
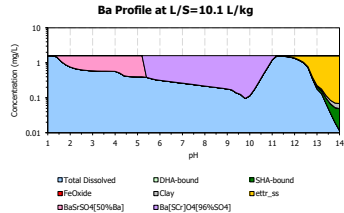
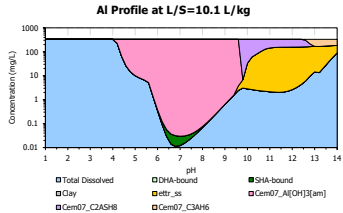
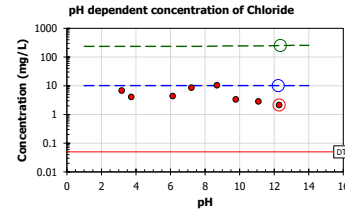
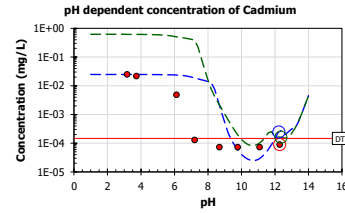
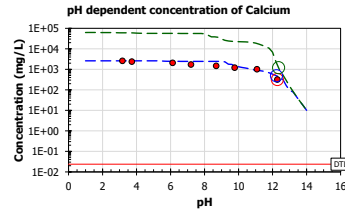
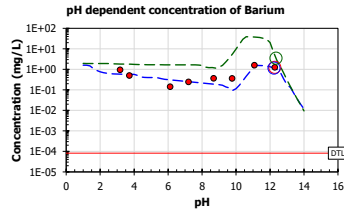
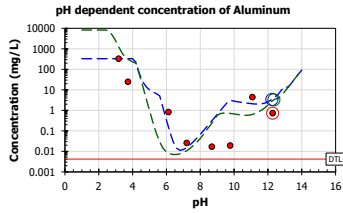
Model Parameters			Available Content								
Entity	Unit	Default	Entity	Unit	Default	Entity	Unit	Default	Entity	Unit	Default
L/S	L/kg	10.08	Ag	mg/kg	1.079E-07	As	mg/kg	9.230	Se	mg/kg	3.477
c0		-5.575	Al	mg/kg	3332	B	mg/kg	332.4	Sn	mg/kg	0.03709
c1		-1.243	Ba	mg/kg	16.12	Hg	mg/kg	0.09999	S	mg/kg	1678
c2		0.4423	Br	mg/kg	0.08702	K	mg/kg	54.70	Sr	mg/kg	320.7
c3		-0.06564	Ca	mg/kg	2.623E+04	Li	mg/kg	9.530	Th	mg/kg	2.320E-07
c4		0.004283	Cd	mg/kg	0.2500	Mg	mg/kg	4730	U	mg/kg	3.630
c5		-0.0001025	Cl	mg/kg	102.0	Mn	mg/kg	97.19	V	mg/kg	39.17
Clay	mg/kg	1.000E+04	Co	mg/kg	2.643	Mo	mg/kg	5.648	Zn	mg/kg	14.74
Hydrous Ferric Oxide	mg/kg	800.0	Cr	mg/kg	10.45	Na	mg/kg	103.5			
Solid Humic Acid	mg/kg	230.7	Cu	mg/kg	6.361	Ni	mg/kg	6.685			
Dissolved Humic Acid	mg/L	2.128	F	mg/kg	94.88	NO3	mg/kg	1000.0			
pe		1.700	Fe	mg/kg	71.15	Pb	mg/kg	0.006376			
pH		12.28	CO32-	mg/kg	173.8	P	mg/kg	728.2			
Extra L/S	L/kg	0.4000	Si	mg/kg	6111	Sb	mg/kg	0.3362			

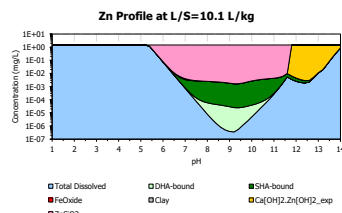
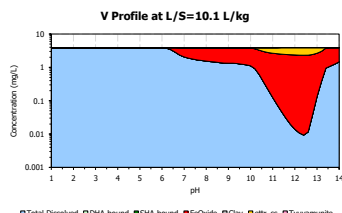
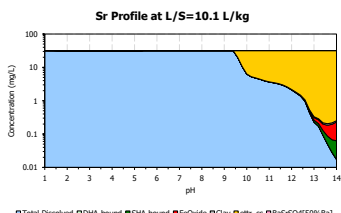
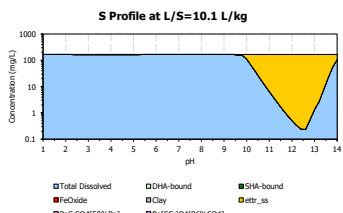
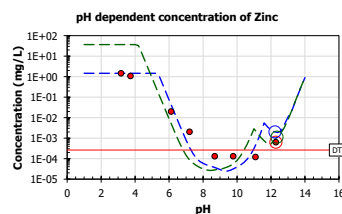
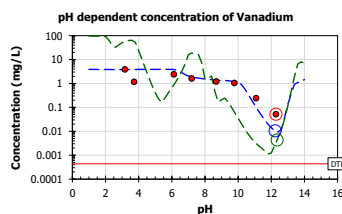
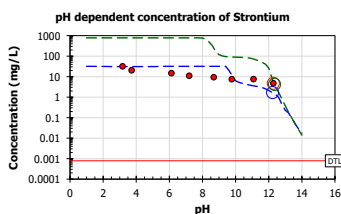
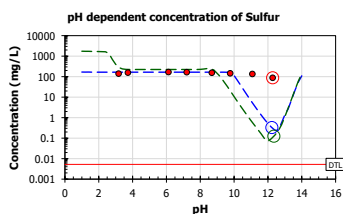
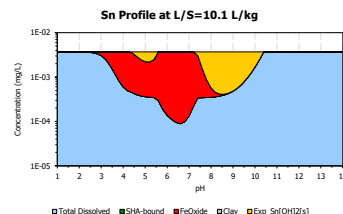
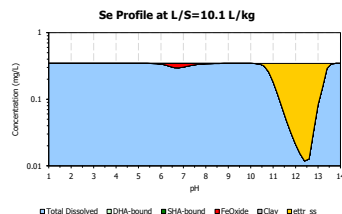
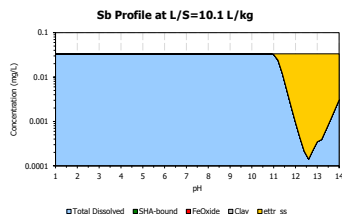
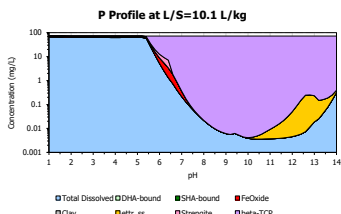
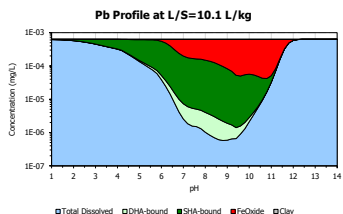
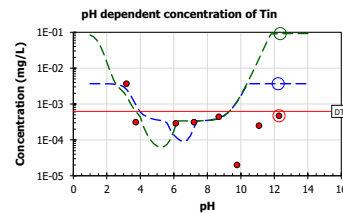
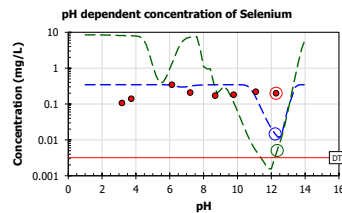
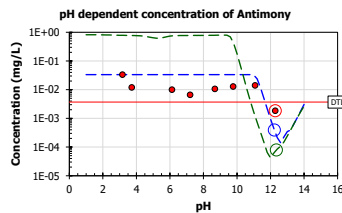
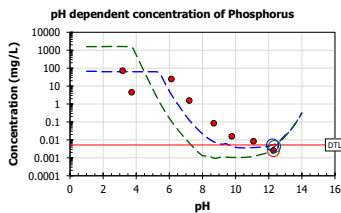
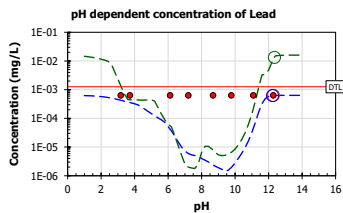
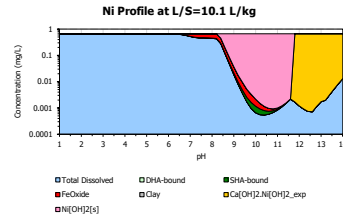
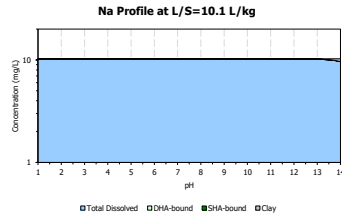
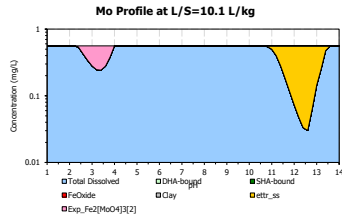
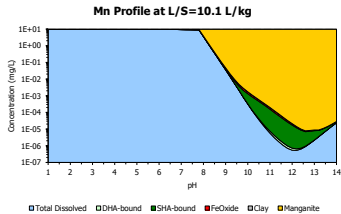
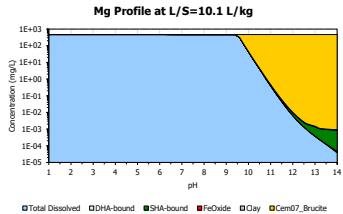
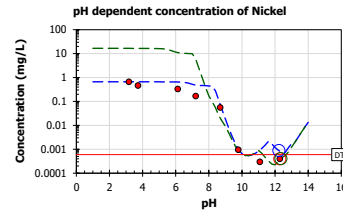
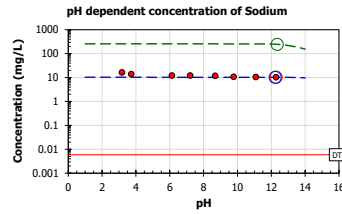
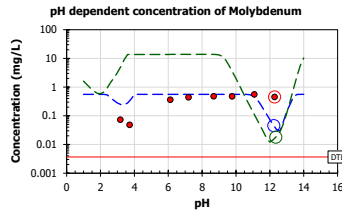
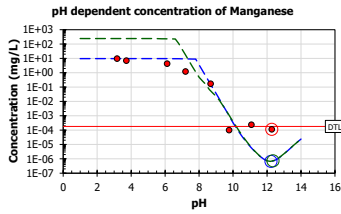
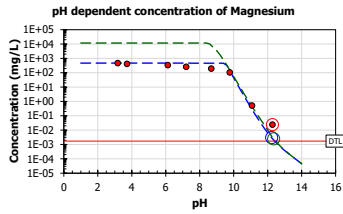
Solid Solutions

Name	End Member	Log(K) Reaction
CShi_ss	Cem07_SiO2[am]_ss	24.21 Cem07_SiO2[am]_ss + 2 H2O -> 1 CShi_ss + 2 H+ + 1 H2SiO4-2
	Cem07_Tob_1_ss	23.87 Cem07_Tob_1_ss -> 1 CShi_ss + 2 Ca+2 + 0.8 H+ + 1.2 H2O + 2.4 H2SiO4-2
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	-35.00 AsO4_Ettringite_ss + 10 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 H3AsO4 + 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	-74.59 BO3_Ettringite_ss + 10 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 3 H3BO3 + 1 ettr_ss
	CO3_Ettringite_ss	-25.67 CO3_Ettringite_ss + 6 H+ + 8 H2O -> 2 Al[OH]4- + 6 Ca+2 + 1 H2CO3 + 2 SO4-2 + 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_ss	-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	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+	Cem07_Gypsum	Yes	4.583	Cem07_Gypsum -> 1 Ca+2 + 2 H2O + 1 SO4-2
B_UO2[OH]2	Yes	-8.329	B_UO2[OH]2 + 2 H+ + 1 e- -> 2 H2O + 1 UO2+	Cem07_Portlandite	Yes	-22.79	Cem07_Portlandite + 2 H+ -> 1 Ca+2 + 2 H2O
Ba[Scr]O4[96%SO4]	Yes	9.790	Ba[Scr]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2	Cr[OH]3[A]	Yes	68.13	Cr[OH]3[A] + 1 H2O -> 1 CrO4-2 + 5 H+ + 3 e-
BaSrSO4[50%Ba]	Yes	8.221	BaSrSO4[50%Ba] -> 0.5 Ba+2 + 1 SO4-2 + 0.5 Sr+2	Exp_Ca[OH]2.Co[OH]2	Yes	-33.22	Exp_Ca[OH]2.Co[OH]2 + 4 H+ -> 1 Ca+2 + 1 Co+2 + 4 H2O
beta-TCP	Yes	28.93	beta-TCP -> 3 Ca+2 + 2 PO4-3	Exp_Ca[OH]2.Cu[OH]2	Yes	-30.00	Exp_Ca[OH]2.Cu[OH]2 + 4 H+ -> 1 Ca+2 + 1 Cu+2 + 4 H2O
Ca[OH]2.Cd[OH]2_exp	Yes	-34.00	Ca[OH]2.Cd[OH]2_exp + 4 H+ -> 1 Ca+2 + 1 Cd+2 + 4 H2O	Exp_Co2SiO4	Yes	5.289	Exp_Co2SiO4 + 2 H+ -> 2 Co+2 + 1 H2SiO4-2
Ca[OH]2.Ni[OH]2_exp	Yes	-32.00	Ca[OH]2.Ni[OH]2_exp + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Ni+2	Exp_Fe2[MoO4]3[2]	Yes	86.35	Exp_Fe2[MoO4]3[2] + 8 H2O -> 2 Fe[OH]4- + 8 H+ + 3 MoO4-2
Ca[OH]2.Pb[OH]2_exp	Yes	-30.00	Ca[OH]2.Pb[OH]2_exp + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Pb+2	Exp_Sn[OH]2[s]	Yes	1.447	Exp_Sn[OH]2[s] + 2 H+ -> 2 H2O + 1 Sn+2
Ca[OH]2.Zn[OH]2_exp	Yes	-30.52	Ca[OH]2.Zn[OH]2_exp + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Zn+2	Fe_Vanadate	Yes	19.18	Fe_Vanadate + 1 H2O -> 0.5 Fe[OH]4- + 1 VO2+ + 0.5 e-
Ca5[OH][AsO4]3[c]	Yes	-35.66	Ca5[OH][AsO4]3[c] + 10 H+ -> 5 Ca+2 + 1 H2O + 3 H3AsO4	Fluorite	Yes	10.96	Fluorite -> 1 Ca+2 + 2 F-
Cd2SiO4	Yes	6.059	Cd2SiO4 + 2 H+ -> 2 Cd+2 + 1 H2SiO4-2	Manganite	Yes	-25.27	Manganite + 3 H+ + 1 e- -> 2 H2O + 1 Mn+2
Cem07_Al[OH]3[am]	Yes	13.76	Cem07_Al[OH]3[am] + 1 H2O -> 1 Al[OH]4- + 1 H+	Ni[OH]2[s]	Yes	-10.80	Ni[OH]2[s] + 2 H+ -> 2 H2O + 1 Ni+2
Cem07_Brucite	Yes	-16.83	Cem07_Brucite + 2 H+ -> 2 H2O + 1 Mg+2	Pb2VO7	Yes	0.9500	Pb2VO7 + 3 H+ -> 1.5 H2O + 1 Pb+2 + 1 VO2+
Cem07_C2ASH8	Yes	17.40	Cem07_C2ASH8 -> 2 Al[OH]4- + 2 Ca+2 + 3 H2O + 1 H2SiO4-2	PbMoO4[c]	Yes	15.80	PbMoO4[c] -> 1 MoO4-2 + 1 Pb+2
Cem07_C2FSH8	Yes	21.41	Cem07_C2FSH8 -> 2 Ca+2 + 2 Fe[OH]4- + 3 H2O + 1 H2SiO4-2	Strengite	Yes	48.00	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
Cem07_C3AH6	Yes	-35.14	Cem07_C3AH6 + 4 H+ -> 2 Al[OH]4- + 3 Ca+2 + 4 H2O	Tenorite	Yes	-7.620	Tenorite + 2 H+ -> 1 Cu+2 + 1 H2O
Cem07_C3FH6	Yes	-30.82	Cem07_C3FH6 + 4 H+ -> 3 Ca+2 + 2 Fe[OH]4- + 4 H2O	Tyuyamunite	Yes	-4.825	Tyuyamunite + 4 H+ + 1 e- -> 0.5 Ca+2 + 2 H2O + 1 UO2+ + 1 VO2+
Cem07_Calcite	Yes	-8.196	Cem07_Calcite + 2 H+ -> 1 Ca+2 + 1 H2CO3	ZnSiO3	Yes	18.69	ZnSiO3 + 1 H2O -> 1 H2SiO4-2 + 1 Zn+2





Model Comparison: residuals - Concentration

Name Alkaline Coal fly ash 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 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	3.17	3.72	6.12	7.20	8.68	9.77	11.1	12.3	Deviation
Al	0.00	1.12	-0.73	-0.22	1.26	2.19	-0.32	0.69	0.37
Ba	-0.21	0.06	0.34	0.01	-0.28	-0.57	-0.08	-0.06	0.09
Br	-	-	-	-	-	-	-	-	-
Ca	0.00	0.04	0.07	0.15	0.22	0.09	-0.05	0.16	0.04
Cd	0.00	0.05	0.69	2.16	1.47	-0.10	-0.40	0.45	0.35
Cl	0.17	0.39	0.36	0.07	-0.01	0.48	0.55	0.67	0.14
Co	0.00	0.20	0.38	0.85	-0.25	-0.08	0.73	1.12	0.21
Cr	-0.26	0.34	1.24	0.18	-0.73	0.05	-0.09	-1.24	0.24
Cu	-0.03	0.33	2.81	1.50	1.37	0.94	0.92	1.37	0.50
F	-	-	-	-	-	-	-	-	-
Fe	-2.91	-0.82	-0.50	1.28	1.56	1.68	1.21	1.75	0.57
CO32-	-	-	-	-	-	-	-	-	-
Si	-0.93	-0.63	-0.29	0.10	0.23	-0.15	0.17	-0.67	0.17
As	0.32	0.44	-0.15	0.09	0.92	0.22	-0.27	-0.46	0.15
B	0.00	0.02	0.04	0.06	0.10	0.17	-0.80	-2.39	0.32
Hg	-	-	-	-	-	-	-	-	-
K	-0.41	-0.14	0.03	-0.21	-0.23	0.34	0.07	0.00	0.08
Li	0.00	0.07	0.10	0.11	0.13	0.16	0.19	0.24	0.05
Mg	0.00	0.06	0.14	0.26	0.38	0.10	-0.27	-0.97	0.14
Mn	0.00	0.14	0.35	0.88	-0.04	0.98	-1.61	-2.23	0.38
Mo	0.54	0.84	0.19	0.10	0.07	0.07	-0.09	-1.04	0.18
Na	-0.21	-0.13	-0.07	-0.07	-0.06	-0.02	-0.01	0.00	0.03
Ni	0.00	0.15	0.29	0.46	0.14	0.03	0.49	0.32	0.10
NO3	-	-	-	-	-	-	-	-	-
Pb	-0.17	-0.25	-1.18	-2.02	-2.42	-2.51	-1.15	-0.01	0.55
P	-0.06	1.14	-0.87	-1.10	-1.03	-0.55	-0.35	0.32	0.28
Sb	0.00	0.44	0.52	0.70	0.49	0.41	0.31	-0.75	0.18
Se	0.51	0.39	-0.02	0.18	0.30	0.28	-0.16	-1.16	0.18
Sn	-0.16	0.49	-0.38	-0.16	-0.03	1.76	1.17	0.89	0.30
S	0.07	0.02	0.00	0.00	0.03	0.04	-1.41	-2.47	0.36
Sr	-0.01	0.18	0.33	0.46	0.53	0.19	-0.33	-0.48	0.13
U	-	-	-	-	-	-	-	-	-
V	-0.01	0.52	0.20	0.07	0.05	0.05	-0.37	-0.71	0.12
Zn	0.00	0.13	0.33	-0.76	-0.55	-0.62	0.56	0.50	0.17
Avg Deviation	0.12	0.09	0.14	0.15	0.15	0.16	0.13	0.20	0.23