



Object Name pH Dependent Leaching Test Model
MSWI Bottom ash NL Reheated 500 C

pH Dependent Leaching Test Scenario



Lab Test

Extra L/S Simulation

Lab Test

Model Parameters

Entity	Unit	Default	Available Content Entity	mg/kg	Entity	mg/kg	Entity	mg/kg
c0		-5.682	Al	5647	Si	1.100E+04	Sb	3.996
c1		-0.7876	As	0.07154	Hg	2.006E-08	Se	0.1612
c2		0.2265	Ba	10.64	K	1083	Sn	0.5723
c3		-0.03096	Ca	4.065E+04	Li	5.222	SO4	8015
c4		0.002052	Cd	2.974	Mg	2371	Sr	102.3
c5		-5.186E-05	Cl	2390	Mn	228.9	V	4.630
Clay	mg/kg	3000	Co	3.056	Mo	1.184	Zn	1307
Hydrous Ferric Oxide	mg/kg	150.0	CO32-	5.002E+04	Na	4191		
L/S	L/kg	10.07	Cr	22.93	Ni	105.8		
pE		4.130	Cu	628.8	Pb	161.9		
pH		10.87	Fe	7388	PO4	468.1		
Solid Humic Acid	mg/kg	60.00	B	41.62				
Simulated Low L/S	L/kg	0.4000						

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

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+
Antimocrandallite-exp	63.00	Antimocrandallite-exp + 8 H2O -> 3 Al[OH]4- + 1 Ca+2 + 3 H+ + 2 Sb[OH]6-
Ba[Scr]O4[96%SO4]	9.790	Ba[Scr]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2
BaSrSO4[50%Ba]	8.221	BaSrSO4[50%Ba] -> 0.5 Ba+2 + 1 SO4-2 + 0.5 Sr+2
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
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
Cerrusite	13.13	Cerrusite -> 1 CO3-2 + 1 Pb+2
Cd2SiO4	6.059	CdSiO4 + 2 H+ -> 2 Cd+2 + 1 H2SiO4-2
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

Name	Log(K)	Reaction
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
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
NiHPO4	25.00	NiHPO4 -> 1 H+ + 1 Ni+2 + 1 PO4-3
PATCH_beta-TCP	28.93	PATCH_beta-TCP -> 3 Ca+2 + 2 PO4-3
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+
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
THERMODDEM_Hydrocalum	-25.34	THERMODDEM_Hydrocalumite[Cr] + 4 H+ -> 2 Al[OH]4- + 4 Ca+2 + 1 CrO4-2 + 13 H2O
Willemite	6.289	Willemite + 2 H+ -> 1 H2SiO4-2 + 2 Zn+2

Model Comparison: residuals - Concentration

Name **MSWI Bottom ash NL Reheated 500 C**

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	3.30	4.31	6.30	7.59	8.37	9.52	10.9	12.0	Deviation
Al	-0.01	-0.05	-0.70	-0.33	0.00	-0.11	-0.11	-0.04	0.10
As	-0.27	-0.26	-2.14	0.21	-0.05	-0.28	-0.12	0.00	0.28
Ba	-0.28	-0.50	-0.48	-0.64	-0.72	-0.80	-0.52	-0.08	0.19
Br	-	-	-	-	-	-	-	-	-
Ca	0.00	0.13	0.10	-0.34	-0.22	-0.14	0.30	0.24	0.08
Cd	0.01	0.18	0.51	1.77	1.70	1.78	-1.00	-1.10	0.50
Cl	-	-	-	-	-	-	-	-	-
Co	0.01	0.31	0.52	1.20	1.22	-0.53	-0.76	-0.92	0.28
CO32-	-	-	-	-	-	-	-	-	-
Cr	-0.01	0.75	0.55	0.10	-0.21	0.63	0.46	0.70	0.18
Cu	-0.22	0.39	1.58	0.38	0.19	0.55	0.87	1.40	0.30
Fe	-0.88	-1.67	0.38	0.48	0.39	0.23	1.05	1.53	0.34
B	-0.74	-0.43	-0.32	-0.20	-0.07	0.52	2.69	1.24	0.39
Si	-0.01	-0.50	-0.87	-0.81	-0.92	-0.40	0.33	1.40	0.27
K	0.01	0.24	0.34	0.39	0.44	0.45	0.48	0.48	0.14
Li	0.01	0.27	-0.25	-0.48	-0.42	-0.32	-0.14	-0.58	0.12
Mg	0.01	0.27	-0.70	-1.16	-1.06	-0.78	0.93	0.08	0.27
Mn	0.01	0.44	-1.45	-1.52	-0.66	-1.38	-2.68	-3.53	0.65
Mo	-1.96	-0.22	0.64	0.29	0.00	0.10	0.14	0.13	0.26
Na	0.01	0.16	0.21	0.24	0.26	0.28	0.32	-0.25	0.08
Ni	0.01	0.13	0.37	0.31	1.11	0.52	-0.12	0.27	0.17
Pb	-1.05	-0.62	1.17	-0.35	-0.23	-1.20	-1.43	-0.83	0.34
PO4	-	-	-	-	-	-	-	-	-
Sb	-0.36	-0.43	-0.88	-0.77	-0.80	-0.68	0.30	-0.07	0.21
Se	0.06	0.03	-0.06	0.12	0.13	0.13	-0.92	-1.62	0.23
Sn	-1.10	-1.23	-1.47	-1.16	-0.73	-0.10	0.55	1.75	0.40
SO4	-	-	-	-	-	-	-	-	-
Sr	0.01	0.17	0.19	-0.25	-0.17	-0.08	-0.03	-0.47	0.08
V	-4.60	-1.72	-0.73	0.35	0.01	0.21	0.95	0.96	0.65
Zn	0.01	0.14	0.43	-0.08	-0.16	0.64	0.89	0.12	0.15
Avg Deviat	0.22	0.13	0.17	0.13	0.13	0.15	0.21	0.23	0.27

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