







Name

Cement mortar TH

pH Dependent Leaching Test Scenario



Lab Test

Extra L/S Simulation

Lab Test

Model Parameters			Available Content								
Entity	Unit	Default	Entity	Unit	Default	Entity	Unit	Default	Entity	Unit	Default
c0		-6.558	Acetic acid	mg/kg	2.220E-07	F	mg/kg	1.900E-08	Pb	mg/kg	4.936
c1		-0.6119	Ag	mg/kg	1.079E-07	Fe	mg/kg	3187	PO4	mg/kg	105.1
c2		0.1720	Al	mg/kg	5102	B	mg/kg	20.04	Sb	mg/kg	0.1892
c3		-0.01929	As	mg/kg	2.509	Si	mg/kg	2639	Se	mg/kg	0.2344
c4		0.0007657	Ba	mg/kg	19.06	Hg	mg/kg	2.006E-07	Sn	mg/kg	0.08675
c5		0	Br	mg/kg	7.990E-08	K	mg/kg	845.3	SO4	mg/kg	7697
Clay	mg/kg	1000	Ca	mg/kg	9.839E+04	Li	mg/kg	2.748	Sr	mg/kg	66.65
Hydrous Ferric Oxide	mg/kg	90.00	Cd	mg/kg	0.2262	Mg	mg/kg	1959	Th	mg/kg	2.320E-07
L/S	L/kg	11.28	Cl	mg/kg	80.16	Mn	mg/kg	63.23	U	mg/kg	2.380E-07
pE		3.950	Co	mg/kg	4.058	Mo	mg/kg	4.383	V	mg/kg	3.805
pH		11.95	CO32-	mg/kg	4.240E+04	Na	mg/kg	149.6	Zn	mg/kg	33.14
Solid Humic Acid	mg/kg	43.99	Cr	mg/kg	18.30	Ni	mg/kg	6.133			
Simulated Low L/S	L/kg	0.4000	Cu	mg/kg	30.35	NO3	mg/kg	6.200E-08			

Name	End Member	Log(K) Reaction
AFhc_ss	Cem07_C4Ac[0_5]H	-40.84 Cem07_C4Ac[0_5]H12_ss + 5 H+ -> 1 AFhc_ss + 2 Al[OH]4- + 0.5 CO3-2 + 4 Ca+2 + 10.5 H2O
	Cem07_C4Fc[0_5]H	-36.87 Cem07_C4Fc[0_5]H12_ss + 5 H+ -> 1 AFhc_ss + 0.5 CO3-2 + 4 Ca+2 + 2 Fe[OH]4- + 10.5 H2O
AFm_ss	Cem07_C4AsH12_ss	-26.72 Cem07_C4AsH12_ss + 4 H+ -> 1 AFm_ss + 2 Al[OH]4- + 4 Ca+2 + 10 H2O + 1 SO4-2
	Cem07_C4FsH12_ss	-22.77 Cem07_C4FsH12_ss + 4 H+ -> 1 AFm_ss + 4 Ca+2 + 2 Fe[OH]4- + 10 H2O + 1 SO4-2
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
CSHi_ss	Cem07_SiO2[am]_s	24.21 Cem07_SiO2[am]_ss + 2 H2O -> 1 CSHi_ss + 2 H+ + 1 H2SiO4-2
	Cem07_Tob_l_ss	23.87 Cem07_Tob_l_ss -> 1 CSHi_ss + 2 Ca+2 + 0.8 H+ + 1.2 H2O + 2.4 H2SiO4-2
CSHi_ss	Cem07_Jenn_ss	-7.799 Cem07_Jenn_ss + 1.33333 H+ -> 1 CSHi_ss + 1.66667 Ca+2 + 1.76667 H2O + 1 H2SiO4-2
	Cem07_Tob_ll_ss	10.36 Cem07_Tob_ll_ss -> 1 CSHi_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
	Li-Ettringite_ss	-5.699 Li-Ettringite_ss + 4 H+ + 8 H2O -> 2 Al[OH]4- + 5 Ca+2 + 2 Li+ + 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				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_Calcite	Yes	8.485	Cem07_Calcite -> 1 CO3-2 + 1 Ca+2
alpha-TCP	Yes	25.50	alpha-TCP -> 3 Ca+2 + 2 PO4-3	Cem07_Gypsum	Yes	4.583	Cem07_Gypsum -> 1 Ca+2 + 2 H2O + 1 SO4-2
Ba[ScR]O4[96%SO4]	Yes	9.790	Ba[ScR]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2	Cem07_Portlandite	Yes	-22.79	Cem07_Portlandite + 2 H+ -> 1 Ca+2 + 2 H2O
Ca[OH]2.Cd[OH]2	Yes	-34.00	Ca[OH]2.Cd[OH]2 + 4 H+ -> 1 Ca+2 + 1 Cd+2 + 4 H2O	CoSiO4	Yes	6.289	CoSiO4 + 2 H+ -> 2 Co+2 + 1 H2SiO4-2
Ca[OH]2.Co[OH]2	Yes	-32.40	Ca[OH]2.Co[OH]2 + 4 H+ -> 1 Ca+2 + 1 Co+2 + 4 H2O	Cr[OH]3[A]	Yes	68.13	Cr[OH]3[A] + 1 H2O -> 1 CrO4-2 + 5 H+ + 3 e-
Ca[OH]2.Cu[OH]2	Yes	-28.52	Ca[OH]2.Cu[OH]2 + 4 H+ -> 1 Ca+2 + 1 Cu+2 + 4 H2O	FeVO4:2H2O_am	Yes	23.48	FeVO4:2H2O_am + 2 H2O -> 1 Fe[OH]4- + 1 VO2+
Ca[OH]2.Ni[OH]2	Yes	-32.00	Ca[OH]2.Ni[OH]2 + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Ni+2	Manganite	Yes	-25.27	Manganite + 3 H+ + 1 e- -> 2 H2O + 1 Mn+2
Ca[OH]2.Pb[OH]2	Yes	-30.00	Ca[OH]2.Pb[OH]2 + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Pb+2	Ni[OH]2[s]	Yes	-10.80	Ni[OH]2[s] + 2 H+ -> 2 H2O + 1 Ni+2
Ca[OH]2.Zn[OH]2	Yes	-30.52	Ca[OH]2.Zn[OH]2 + 4 H+ -> 1 Ca+2 + 4 H2O + 1 Zn+2	Pb[OH]2[C]	Yes	-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
Ca2Cd[PO4]2	Yes	32.95	Ca2Cd[PO4]2 -> 2 Ca+2 + 1 Cd+2 + 2 PO4-3	Pb2V2O7	Yes	0.9500	Pb2V2O7 + 3 H+ -> 1.5 H2O + 1 Pb+2 + 1 VO2+
Ca4Cd[PO4]3OH	Yes	39.23	Ca4Cd[PO4]3OH + 1 H+ -> 4 Ca+2 + 1 Cd+2 + 1 H2O + 3 PO4-3	Pb3[VO4]2	Yes	-3.070	Pb3[VO4]2 + 4 H+ -> 2 H2O + 1.5 Pb+2 + 1 VO2+
Ca5[OH][AsO4]3[c]	Yes	26.13	Ca5[OH][AsO4]3[c] + 1 H+ -> 3 AsO4-3 + 5 Ca+2 + 1 H2O	PbMoO4[c]	Yes	15.80	PbMoO4[c] -> 1 MoO4-2 + 1 Pb+2
Cem07_Al[OH]3[am]	Yes	13.76	Cem07_Al[OH]3[am] + 1 H2O -> 1 Al[OH]4- + 1 H+	Sn[OH]2[s]	Yes	1.447	Sn[OH]2[s] + 2 H+ -> 2 H2O + 1 Sn+2
Cem07_Brucite	Yes	-16.83	Cem07_Brucite + 2 H+ -> 2 H2O + 1 Mg+2	Strenigite	Yes	48.00	Strenigite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
Cem07_C2ASH8	Yes	17.40	Cem07_C2ASH8 -> 2 Al[OH]4- + 2 Ca+2 + 3 H2O + 1 H2SiO4-2	Tenorite	Yes	-7.620	Tenorite + 2 H+ -> 1 Cu+2 + 1 H2O
Cem07_C2FSH8	Yes	21.41	Cem07_C2FSH8 -> 2 Ca+2 + 2 Fe[OH]4- + 3 H2O + 1 H2SiO4-2	Willemite	Yes	6.289	Willemite + 2 H+ -> 1 H2SiO4-2 + 2 Zn+2

Model Comparison: residuals - Concentration

Sample

Name Cement mortar TH

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	2	3	1	Total Avg
pH	2.10	5.10	7.10	9.20	11.6	12.0	12.1	12.9	Deviation
Al	0.00	0.21	-0.76	2.40	0.68	0.21	-0.24	0.25	0.33
As	-0.14	1.19	0.91	-0.43	-1.89	-0.98	-1.37	-0.08	0.37
Ba	-0.01	-0.63	-0.97	-0.91	0.08	0.16	0.00	-0.01	0.18
Ca	0.00	0.03	-0.05	0.01	0.08	0.71	0.06	0.08	0.09
Cd	0.00	0.84	0.61	-1.34	1.16	0.20	-0.28	-0.40	0.26
Cl	-1.22	-1.26	-1.11	-1.16	-1.15	-0.03	-1.04	-0.07	0.36
Co	0.00	0.79	1.50	0.10	0.42	-0.20	-0.40	-0.17	0.23
CO32-	-	-	-	-	-	-	-	-	-
Cr	-0.01	-0.13	-0.09	0.14	-0.93	0.11	-0.62	-0.07	0.14
Cu	0.00	1.88	1.24	0.33	0.02	-0.24	-0.29	0.57	0.30
Fe	-0.01	1.31	-0.28	0.41	1.17	0.89	-0.46	0.70	0.27
B	0.28	-0.01	0.69	1.01	0.02	0.02	-0.11	-1.32	0.23
Si	0.00	0.79	0.79	0.94	-0.29	-0.64	-0.85	-0.22	0.23
K	-0.35	-0.33	-0.24	-0.27	-0.32	-0.03	-0.27	-0.11	0.09
Li	0.00	0.08	0.15	0.26	0.07	0.10	0.04	-0.50	0.08
Mg	0.00	0.16	0.66	1.04	-1.11	0.22	-1.17	-0.69	0.27
Mn	0.00	2.05	3.19	0.02	-3.21	-3.27	-3.42	-3.39	0.96
Mo	0.21	0.43	-0.29	0.06	-0.42	0.56	-0.23	0.53	0.13
Na	0.02	-1.15	-0.48	-0.87	0.08	-0.03	0.05	-2.48	0.36
Ni	0.00	0.52	1.28	0.38	0.52	-0.17	-0.26	0.33	0.20
Pb	-0.15	0.71	0.24	0.24	0.56	0.58	0.63	1.17	0.22
PO4	-	-	-	-	-	-	-	-	-
Sb	0.08	0.30	0.02	0.53	-0.78	-1.09	-1.18	-0.22	0.24
Se	0.00	0.15	0.05	0.38	-0.91	-0.63	-0.65	0.29	0.17
Sn	0.00	-0.27	-0.29	-0.07	1.07	1.07	1.07	1.07	0.27
SO4	0.15	0.03	0.17	0.34	-1.42	-0.22	-0.57	-0.46	0.21
Sr	0.00	0.05	0.10	0.15	0.20	0.24	0.17	-0.64	0.09
V	-1.36	-0.60	0.08	0.34	0.72	0.78	0.88	2.30	0.39
Zn	0.00	1.05	1.97	1.70	-0.11	-0.97	-0.58	0.07	0.38
Avg Deviation	0.07	0.16	0.19	0.16	0.19	0.16	0.18	0.20	0.26