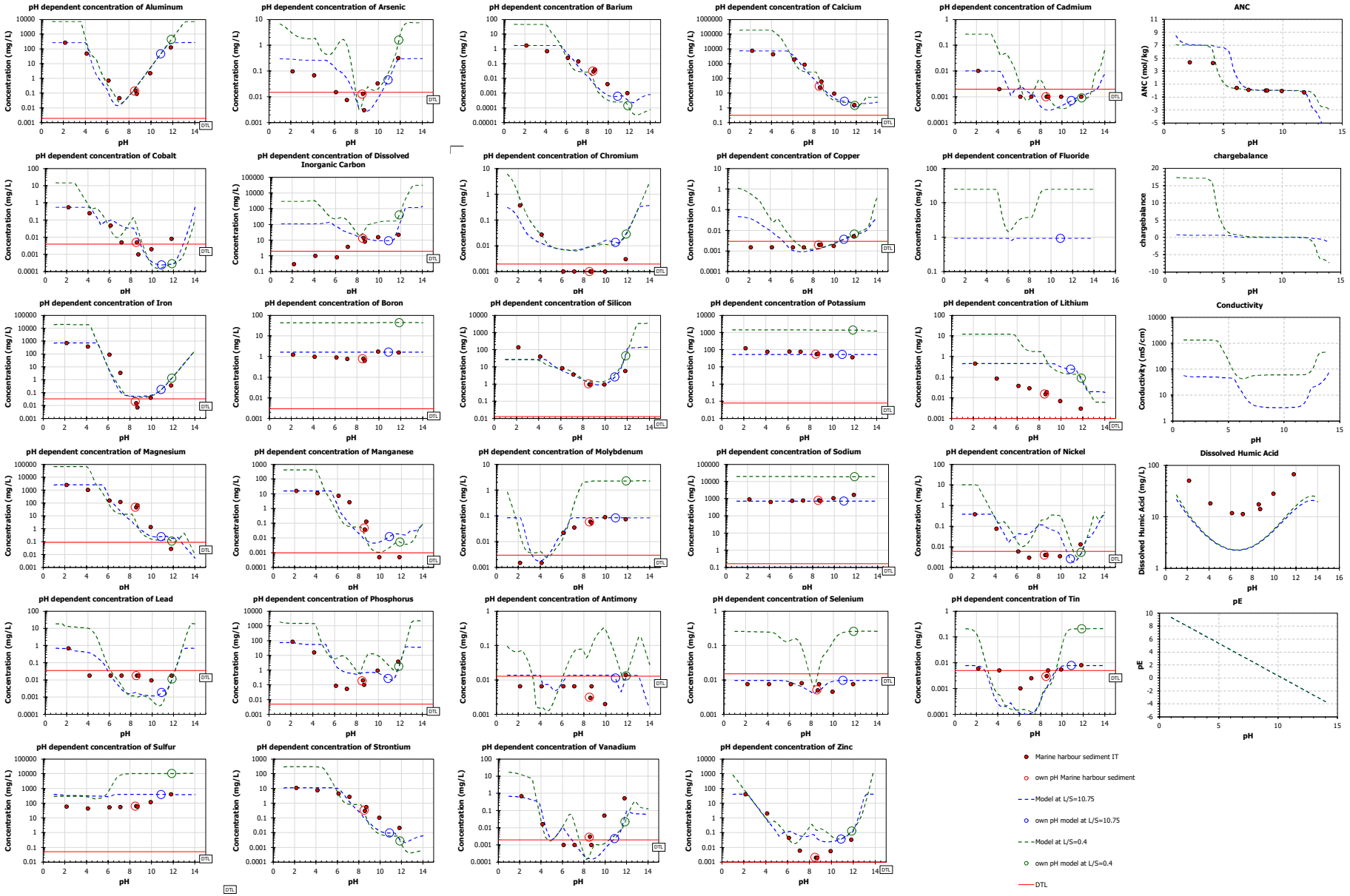
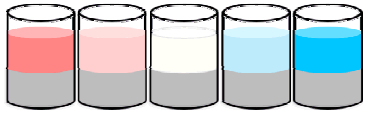
MARINE HARBOUR SEDIMENT IT

COMPARISON pH DEPENDENCE WITH MODEL



Object pH Dependent Leaching Test Model
Name Marine harbour sediment IT

pH Dependent Leaching Test Scenario



Lab Test

Extra L/S Simulation

Lab Test

Model Parameters

Entity	Unit	Default
c0		-4.620
c1		-0.3602
c2		0.02238
c3		-0.001288
c4		0.0003533
c5		-1.815E-05
Clay	mg/kg	3000
Hydrous Ferric Oxic	mg/kg	1700
L/S	L/kg	10.75
pE		1.710
pH		8.641
Solid Humic Acid	mg/kg	1224
Simulated Low L/S	L/kg	0.4000

Available Content

Entity	mg/kg	Entity	mg/kg	Entity	mg/kg
Al	2895	B	17.64	PO4	2749
As	3.300	Si	1506	Sb	0.1462
Ba	18.54	Hg	2.006E-07	Se	0.1038
Ca	8.060E+04	K	565.0	Sn	0.08355
Cd	0.1088	Li	4.886	SO4	1.244E+04
Cl	1500	Mg	2.695E+04	Sr	117.3
Co	5.899	Mn	167.5	V	7.376
CO32-	1.844E+05	Mo	0.9057	Zn	435.3
Cr	3.972	Na	7764		
Cu	0.5200	Ni	4.092		
F	10.00	NO3	6.200E-08		
Fe	7618	Pb	7.389		

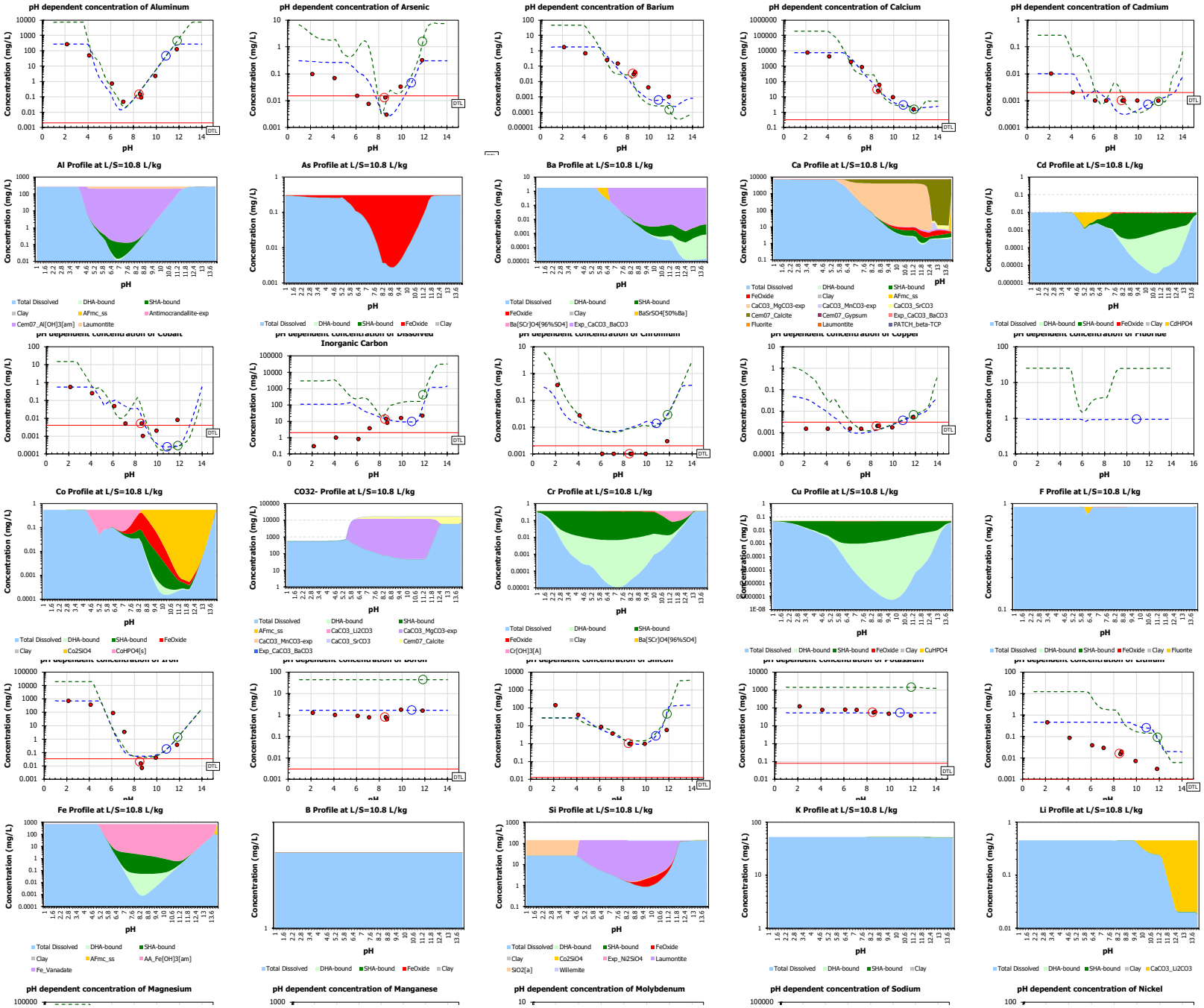
Solid Solutions

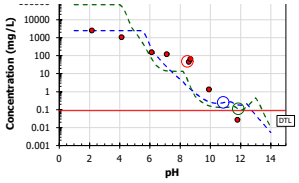
Name	End Member	Log(K)	Reaction
AFmc_ss	Cem07_C4AcH11_ss	-24.50	Cem07_C4AcH11_ss + 4 H+ -> 1 AFmc_ss + 2 Al[OH]4- + 1 CO3-2 + 4 Ca+2 + 9 H2O
	Cem07_C4FcH12_ss	-20.47	Cem07_C4FcH12_ss + 4 H+ -> 1 AFmc_ss + 1 CO3-2 + 4 Ca+2 + 2 Fe[OH]4- + 10 H2O

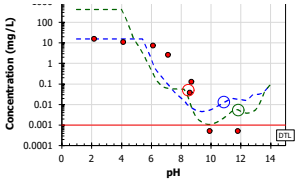
Minerals

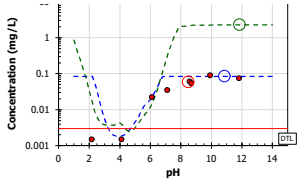
Name	Log(K)	Reaction
AA_Fe[OH]3[am]	16.60	AA_Fe[OH]3[am] + 1 H2O -> 1 Fe[OH]4- + 1 H+
Antimocrandallite-e	63.00	Antimocrandallite-exp + 8 H2O -> 3 Al[OH]4- + 1 Ca+2 + 3 H+ + 2 Sb[OH]6-
Ba[SCr]O4[96%SO4	9.790	Ba[SCr]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2
BaSrSO4[50%Ba]	8.221	BaSrSO4[50%Ba] -> 0.5 Ba+2 + 1 SO4-2 + 0.5 Sr+2
Ca[OH]Sb[OH]6_exp	4.000	Ca[OH]Sb[OH]6_exp + 1 H+ -> 1 Ca+2 + 1 H2O + 1 Sb[OH]6-
CaCO3_Li2CO3	21.30	CaCO3_Li2CO3 -> 2 CO3-2 + 1 Ca+2 + 2 Li+
CaCO3_MgCO3-exp	18.02	CaCO3_MgCO3-exp -> 2 CO3-2 + 1 Ca+2 + 1 Mg+2
CaCO3_MnCO3-exp	20.78	CaCO3_MnCO3-exp -> 2 CO3-2 + 1 Ca+2 + 1 Mn+2
CaCO3_SrCO3	19.85	CaCO3_SrCO3 -> 2 CO3-2 + 1 Ca+2 + 1 Sr+2
CaSb[OH]6[s]2_exp	19.41	CaSb[OH]6[s]2_exp -> 1 Ca+2 + 2 Sb[OH]6-
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_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
Co2SiO4	6.289	Co2SiO4 + 2 H+ -> 2 Co+2 + 1 H2SiO4-2
CoHPO4[s]	24.48	CoHPO4[s] -> 1 Co+2 + 1 H+ + 1 PO4-3
Cr[OH]3[A]	68.13	Cr[OH]3[A] + 1 H2O -> 1 CrO4-2 + 5 H+ + 3 e-

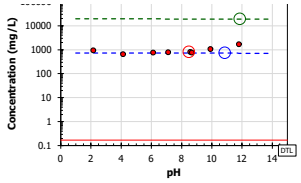
Name	Log(K)	Reaction
CuHPO4	26.00	CuHPO4 -> 1 Cu+2 + 1 H+ + 1 PO4-3
Exp_CaCO3_B	21.30	Exp_CaCO3_BaCO3 -> 1 Ba+2 + 2 CO3-2 + 1 Ca+2
Exp_Ni2SiO4	5.498	Exp_Ni2SiO4 + 2 H+ -> 1 H2SiO4-2 + 2 Ni+2
Fe_Vanadate	19.18	Fe_Vanadate + 1 H2O -> 0.5 Fe[OH]4- + 1 VO2+ + 0.5 e-
Fe2[MoO4]3[2	86.35	Fe2[MoO4]3[2] + 8 H2O -> 2 Fe[OH]4- + 8 H+ + 3 MoO4-2
Fluorite	10.96	Fluorite -> 1 Ca+2 + 2 F-
Laumontite	118.0	Laumontite + 8 H2O -> 2 Al[OH]4- + 1 Ca+2 + 8 H+ + 4 H2SiO4-2
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-T	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
PbMoO4[c]	15.80	PbMoO4[c] -> 1 MoO4-2 + 1 Pb+2
PbOH[Sb[OH]	12.00	PbOH[Sb[OH]6]_exp1 + 1 H+ -> 1 H2O + 1 Pb+2 + 1 Sb[OH]6-
Sb[OH]3[s]	32.89	Sb[OH]3[s] + 3 H2O -> 3 H+ + 1 Sb[OH]6- + 2 e-
SiO2[a]	24.64	SiO2[a] + 2 H2O -> 2 H+ + 1 H2SiO4-2
Willemite	6.289	Willemite + 2 H+ -> 1 H2SiO4-2 + 2 Zn+2
ZnHPO4	24.48	ZnHPO4 -> 1 H+ + 1 PO4-3 + 1 Zn+2

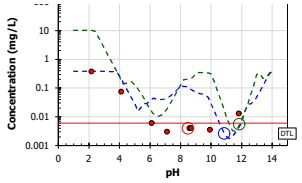

pH dependent concentration of Aluminum
pH dependent concentration of Arsenic
pH dependent concentration of Barium
pH dependent concentration of Calcium
pH dependent concentration of Cadmium
Al Profile at L/S=10.8 L/kg
As Profile at L/S=10.8 L/kg
Ba Profile at L/S=10.8 L/kg
Ca Profile at L/S=10.8 L/kg
Cd Profile at L/S=10.8 L/kg
pH dependent concentration of Cobalt
pH dependent concentration of Dissolved Inorganic Carbon
pH dependent concentration of Chromium
pH dependent concentration of Copper
pH dependent concentration of Fluoride
Co Profile at L/S=10.8 L/kg
CO32- Profile at L/S=10.8 L/kg
Cr Profile at L/S=10.8 L/kg
Cu Profile at L/S=10.8 L/kg
F Profile at L/S=10.8 L/kg
pH dependent concentration of Iron
pH dependent concentration of Boron
pH dependent concentration of Silicon
pH dependent concentration of Potassium
pH dependent concentration of Lithium
Fe Profile at L/S=10.8 L/kg
B Profile at L/S=10.8 L/kg
Si Profile at L/S=10.8 L/kg
K Profile at L/S=10.8 L/kg
Li Profile at L/S=10.8 L/kg
pH dependent concentration of Magnesium
pH dependent concentration of Manganese
pH dependent concentration of Molybdenum
pH dependent concentration of Sodium
pH dependent concentration of Nickel
Concentration (mg/L)
pH
DTL
Total Dissolved
DHA-bound
SHA-bound
FeOxide
Clay
AFmc_ss
Antimocrandallite-exp
Cem07_Al[OH]3[am]
Laumontite
CaCO3_MgCO3-exp
CaCO3_MnCO3-exp
CaCO3_SrCO3
Cem07_Calcite
Cem07_Gypsum
Exp_CaCO3_BaCO3
Fluorite
PATCH_beta-TCP
BaSrSO4[50%Ba]
Ba[SCr]O4[96%SO4]
Exp_CaCO3_BaCO3
CdHPO4
CaCO3_Li2CO3
Co2SiO4
CoHPO4[s]
Cr[OH]3[A]
CuHPO4
Fe_Vanadate
AA_Fe[OH]3[am]
Exp_Ni2SiO4
SiO2[a]
Willemite



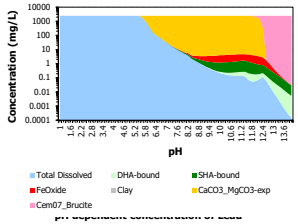




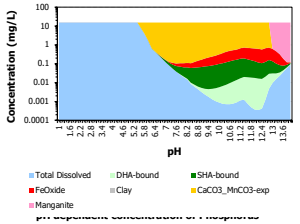




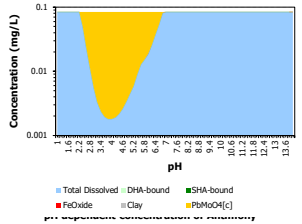
Mg Profile at L/S=10.8 L/kg



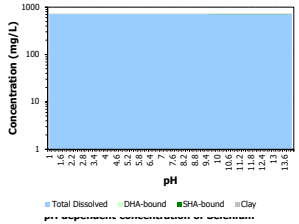
Mn Profile at L/S=10.8 L/kg



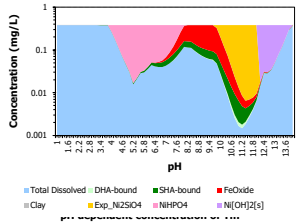
Mo Profile at L/S=10.8 L/kg

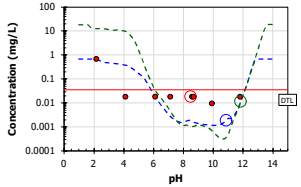


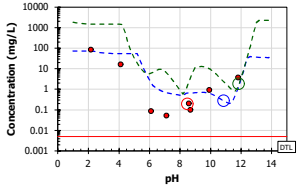
Na Profile at L/S=10.8 L/kg

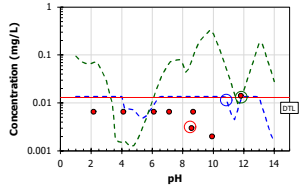


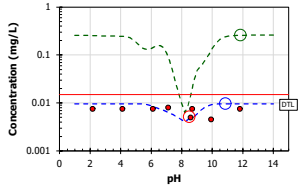
Ni Profile at L/S=10.8 L/kg

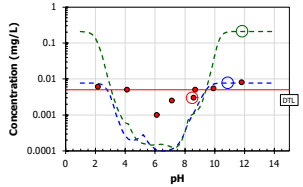




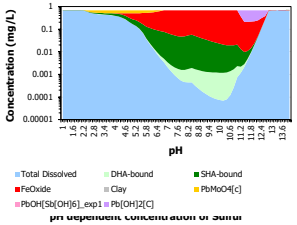




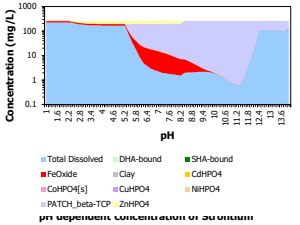




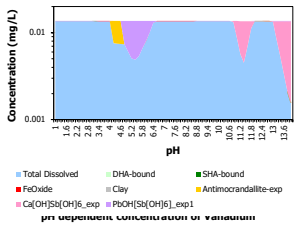
Pb Profile at L/S=10.8 L/kg



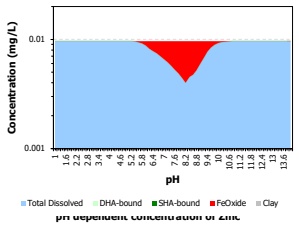
PO4 Profile at L/S=10.8 L/kg



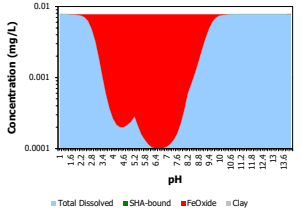
Sb Profile at L/S=10.8 L/kg

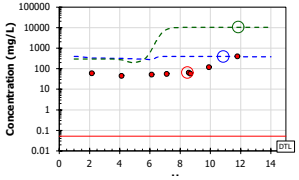


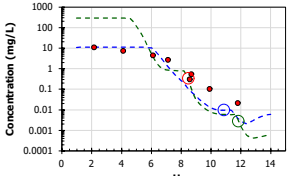
Se Profile at L/S=10.8 L/kg

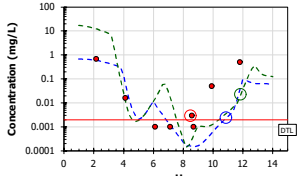


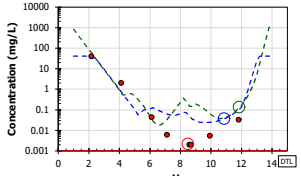
Sn Profile at L/S=10.8 L/kg



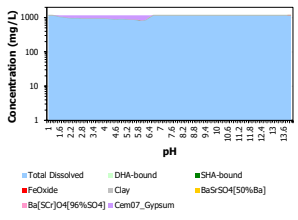




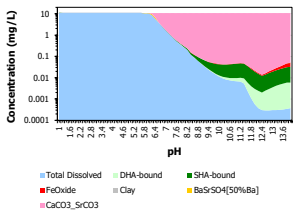




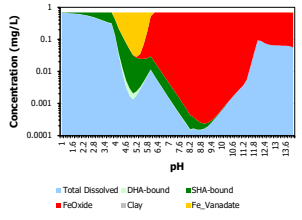
SO4 Profile at L/S=10.8 L/kg



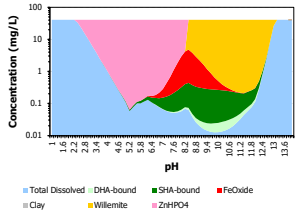
Sr Profile at L/S=10.8 L/kg



V Profile at L/S=10.8 L/kg



Zn Profile at L/S=10.8 L/kg



Model Comparison: residuals - Concentration

Name **Marine harbour sediment IT**

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*	*3*	*4*	*2*	*1*	*Total Avg*
pH	*2.16*	*4.13*	*6.12*	*7.12*	*8.58*	*8.70*	*9.92*	*11.8*	*Deviation*
Al	0.01	0.54	-0.85	-0.46	0.20	0.55	0.35	0.27	0.17
As	0.47	0.59	0.91	0.83	-0.62	-0.01	-0.59	-0.05	0.21
Ba	0.01	0.40	0.25	-0.34	-0.81	-1.03	-0.74	-0.44	0.21
Ca	0.00	0.24	0.24	-0.29	0.11	-0.38	-0.31	-0.16	0.09
Cd	0.00	0.69	0.38	0.11	-0.51	-0.52	-0.36	0.04	0.14
Cl	-	-	-	-	-	-	-	-	-
Co	0.01	0.34	0.33	0.96	0.38	0.88	-0.71	-1.48	0.27
CO32-	-	-	-	-	-	-	-	-	-
Cr	-0.62	-0.34	0.85	0.84	0.98	1.00	1.20	0.98	0.31
Cu	1.38	0.75	-0.15	-0.20	-0.18	-0.16	0.11	0.06	0.20
F	-	-	-	-	-	-	-	-	-
Fe	0.00	0.29	-1.27	-1.46	0.55	0.88	0.19	0.52	0.28
B	0.12	0.22	0.26	0.33	0.32	0.42	-0.03	0.02	0.09
Si	-0.71	-0.16	-0.14	-0.04	0.12	0.09	0.01	0.91	0.15
Hg	-	-	-	-	-	-	-	-	-
K	-0.36	-0.15	-0.17	-0.15	-0.01	-0.05	0.06	0.16	0.06
Li	0.01	0.73	1.08	1.19	1.48	1.38	1.68	1.45	0.43
Mg	0.01	0.39	0.19	-0.70	-1.43	-1.68	-0.68	0.83	0.32
Mn	0.01	0.16	-0.90	-1.45	-0.68	-1.27	1.03	1.57	0.37
Mo	1.75	0.10	0.01	0.38	0.15	0.20	-0.03	0.06	0.23
Na	-0.10	0.05	-0.01	-0.03	-0.04	-0.02	-0.17	-0.37	0.05
Ni	0.00	0.42	0.83	1.18	1.38	1.34	1.01	-0.49	0.34
Pb	-0.01	1.32	0.00	-0.79	-1.03	-1.05	-0.90	-0.26	0.29
PO4	-	-	-	-	-	-	-	-	-
Sb	0.32	0.16	0.15	0.32	0.66	0.32	0.83	-0.09	0.15
Se	0.11	0.11	0.05	-0.10	-0.03	-0.18	0.31	0.11	0.05
Sn	0.10	-1.34	-0.97	-1.35	-0.42	-0.55	0.12	-0.01	0.28
SO4	-	-	-	-	-	-	-	-	-
Sr	0.01	0.17	0.32	-0.33	-0.52	-0.86	-0.87	-0.73	0.20
Th	-	-	-	-	-	-	-	-	-
U	-	-	-	-	-	-	-	-	-
V	-0.06	0.56	0.94	0.08	-1.29	-0.82	-1.95	-1.10	0.37
Zn	0.01	-0.44	0.45	1.02	1.39	1.31	0.65	0.47	0.30
Avg Deviati	0.10	0.11	0.12	0.15	0.16	0.17	0.16	0.14	0.22

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