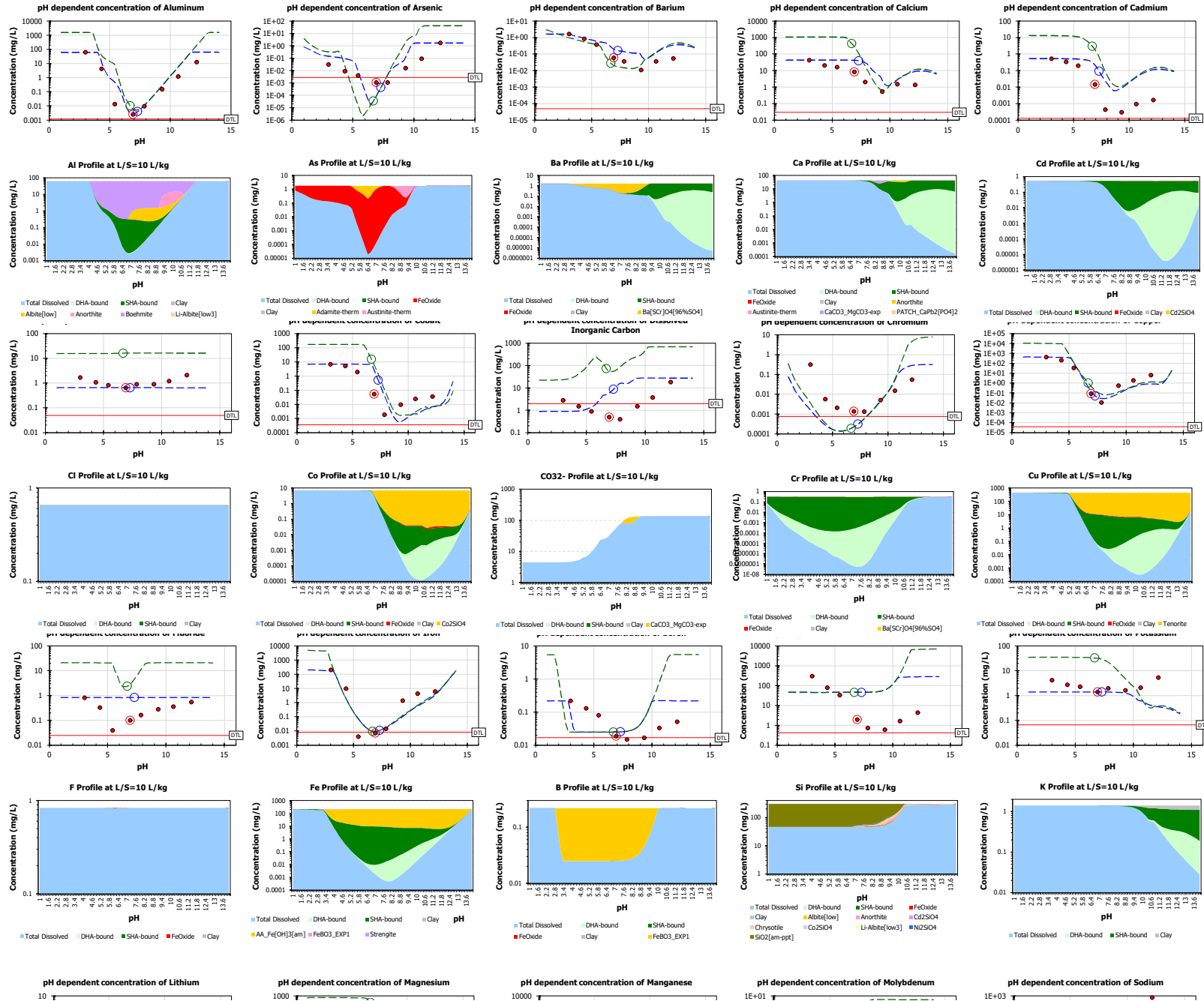
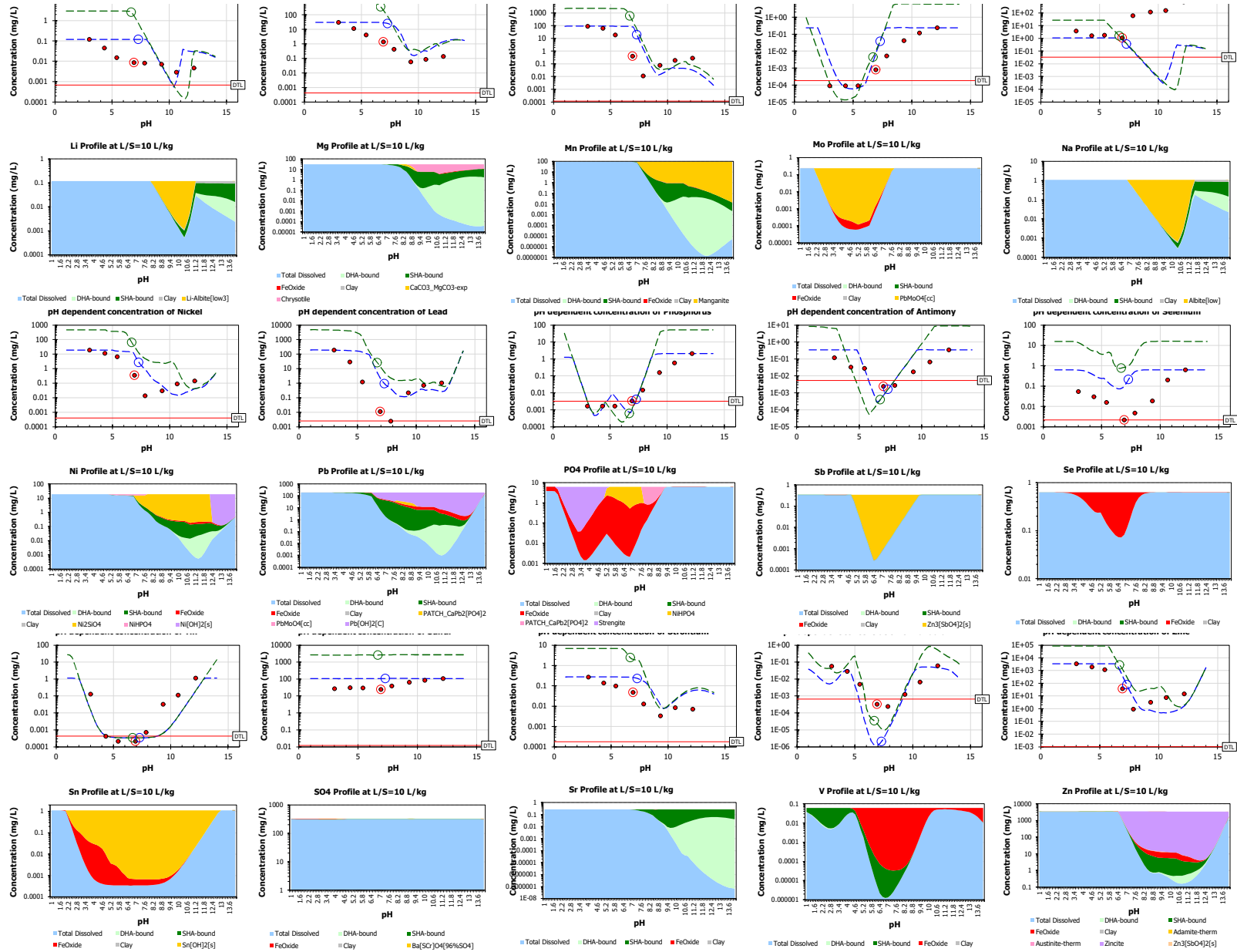


● Zinc\_Soil    
 ○ own pH Zn soil    
 — Model at L/S=10    
 ○ own pH model at L/S=10    
 - - - Model at L/S=0.4    
 ○ own pH model at L/S=0.4    
— DTL



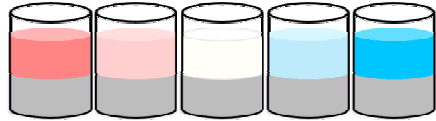
NATURAL Zn CONTAMINATED SOIL

COMPARISON AND PARTITIONING



**Object Name**      **Model input**      **Chemical speciation Fingerprint**  
 Natural Zn contaminated soil

**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		-5.365	Al	634.9	Fe	2110	Pb	1934
c1		0.9994	As	17.51	B	2.204	PO4	63.36
c2		-0.6840	Ba	16.58	Si	3039	Sb	3.485
c3		0.1213	Br	7.990E-08	Hg	2.006E-07	Se	6.299
c4		-0.008092	Ca	438.5	K	14.04	Sn	11.26
c5		0.0001843	Cd	5.399	Li	1.198	SO4	3242
Clay	mg/kg	5000	Cl	6.548	Mg	301.9	Sr	2.734
Hydrous Ferric Oxid	mg/kg	1250	Co	69.95	Mn	910.9	Th	2.320E-07
L/S	L/kg	10.02	CO32-	1380	Mo	2.400	U	2.380E-07
pE		7.680	Cr	3.180	Na	10.95	V	0.6169
pH		6.920	Cu	4398	Ni	188.8	Zn	3.450E+04
Solid Humic Acid	mg/kg	6019	F	8.359	NO3	6.200E-08		
Simulated Low L/S	L/kg	0.4000						

**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+	Fluorite	10.96	Fluorite -> 1 Ca+2 + 2 F-
Adamite-therm	12.64	Adamite-therm + 1 H+ -> 1 AsO4-3 + 1 H2O + 2 Zn+2	Li-Albite[low3]	84.48	Li-Albite[low3] + 8 H2O -> 1 Al[OH]4- + 6 H+ + 3 H2SiO4-2 + 1 Li+
Albite[low]	85.27	Albite[low] + 8 H2O -> 2 Al[OH]4- + 6 H+ + 3 H2SiO4-2 + 1 Na+	Manganite	-25.27	Manganite + 3 H+ + 1 e- -> 2 H2O + 1 Mn+2
Anorthite	63.81	Anorthite + 8 H2O -> 2 Al[OH]4- + 1 Ca+2 + 4 H+ + 2 H2SiO4-2	Ni[OH]2[s]	-10.80	Ni[OH]2[s] + 2 H+ -> 2 H2O + 1 Ni+2
Austinite-therm	11.47	Austinite-therm + 1 H+ -> 1 AsO4-3 + 1 Ca+2 + 1 H2O + 1 Zn+2	Ni2SiO4	5.498	Ni2SiO4 + 2 H+ -> 1 H2SiO4-2 + 2 Ni+2
Ba[SCr]O4[96%SO4]	9.790	Ba[SCr]O4[96%SO4] -> 1 Ba+2 + 0.04 CrO4-2 + 0.96 SO4-2	NiHPO4	25.00	NiHPO4 -> 1 H+ + 1 Ni+2 + 1 PO4-3
BaSrSO4[50%Ba]	8.221	BaSrSO4[50%Ba] -> 0.5 Ba+2 + 1 SO4-2 + 0.5 Sr+2	Pb[OH]2[C]	-8.150	Pb[OH]2[C] + 2 H+ -> 2 H2O + 1 Pb+2
Boehmite	14.42	Boehmite + 2 H2O -> 1 Al[OH]4- + 1 H+	PbMoO4[cc]	13.36	PbMoO4[cc] -> 1 MoO4-2 + 1 Pb+2
CaCO3_MgCO3-exp	18.02	CaCO3_MgCO3-exp -> 2 CO3-2 + 1 Ca+2 + 1 Mg+2	SiO2[am-ppt]	24.40	SiO2[am-ppt] + 2 H2O -> 2 H+ + 1 H2SiO4-2
Cem07_Calcite	8.485	Cem07_Calcite -> 1 CO3-2 + 1 Ca+2	Sn[OH]2[s]	1.447	Sn[OH]2[s] + 2 H+ -> 2 H2O + 1 Sn+2
Cem07_Gypsum	4.583	Cem07_Gypsum -> 1 Ca+2 + 2 H2O + 1 SO4-2	Strengite	48.00	Strengite + 2 H2O -> 1 Fe[OH]4- + 4 H+ + 1 PO4-3
Chrysotile	10.45	Chrysotile + 2 H+ -> 1 H2O + 2 H2SiO4-2 + 3 Mg+2	Tenorite	-7.620	Tenorite + 2 H+ -> 1 Cu+2 + 1 H2O
Co2SiO4	6.289	Co2SiO4 + 2 H+ -> 2 Co+2 + 1 H2SiO4-2	Zincite	-11.14	Zincite + 2 H+ -> 1 H2O + 1 Zn+2
Fe_Vanadate	19.18	Fe_Vanadate + 1 H2O -> 0.5 Fe[OH]4- + 1 VO2+ + 0.5 e-	Zn3[SbO4]2[s]	3.000	Zn3[SbO4]2[s] + 4 H+ + 4 H2O -> 2 Sb[OH]6- + 3 Zn+2
FeBO3_EXP1	31.48	FeBO3_EXP1 + 2 H2O -> 1 Fe[OH]4- + 2 H+ + 1 H2BO3-			

**Model Comparison: residuals - Concentration**

**Name** Natural Zn contaminated soil

**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	3.00	4.33	5.41	6.92	7.84	9.32	10.6	12.2	Deviation	
Al	0.00	0.49	1.54	0.03	0.05	0.26	0.66	0.70	0.24	
As	0.67	1.01	0.38	-1.08	0.59	0.91	1.27	0.00	0.29	
B	-0.38	-0.72	-0.51	0.12	0.25	0.59	0.82	0.63	0.19	
Ba	0.00	0.03	0.21	0.53	0.58	0.89	0.51	0.80	0.19	
Br	-	-	-	-	-	-	-	-	-	
Ca	0.00	0.33	0.43	0.70	1.18	0.70	0.28	0.80	0.23	
Cd	0.00	0.19	0.40	1.17	1.74	1.47	1.62	1.84	0.45	
Cl	-0.42	-0.22	-0.11	0.00	-0.14	-0.14	-0.27	-0.51	0.10	
Co	0.00	0.13	0.54	1.73	1.37	-1.20	-1.05	-0.74	0.36	
CO32-	-	-	-	-	-	-	-	-	-	
Cr	-2.30	-1.32	-1.17	-0.78	-0.37	-0.04	0.55	0.72	0.39	
Cu	-0.02	0.28	0.52	0.22	0.40	-0.80	-0.64	-0.90	0.19	
F	0.00	0.40	1.32	0.92	0.71	0.47	0.36	0.18	0.24	
Fe	-0.07	-0.72	1.26	0.11	0.08	-1.12	-0.87	-0.25	0.26	
Hg	-	-	-	-	-	-	-	-	-	
K	-0.47	-0.29	-0.21	0.00	-0.15	-0.11	-0.54	-1.19	0.18	
Li	0.00	0.42	0.90	1.14	1.15	-0.06	-0.39	0.81	0.26	
Mg	0.00	0.42	0.85	1.31	1.63	0.54	0.57	1.01	0.33	
Mn	0.00	0.17	0.69	2.29	2.16	-0.74	-0.62	-0.96	0.44	
Mo	1.49	-0.09	-0.13	0.94	1.66	0.76	0.30	0.00	0.32	
Na	-0.54	-0.17	-0.22	-0.12	-2.78	-4.55	-5.39	-3.43	1.04	
Ni	0.00	0.22	0.39	1.40	1.83	0.36	-0.78	-0.54	0.32	
NO3	-	-	-	-	-	-	-	-	-	
Pb	-0.01	0.77	2.05	2.30	2.23	-0.23	-0.29	-0.59	0.49	
PO4	-	-	-	-	-	-	-	-	-	
Sb	0.45	1.01	-0.03	-0.55	0.32	1.00	0.71	0.00	0.22	
Se	1.05	1.07	1.05	1.66	2.03	1.52	0.50	0.00	0.45	
Si	-0.82	-0.23	0.13	1.37	1.80	2.00	2.20	1.80	0.53	
Sn	-0.96	0.05	0.21	0.20	-0.32	-1.72	-1.27	-0.75	0.31	
SO4	-	-	-	-	-	-	-	-	-	
Sr	0.00	0.30	0.44	0.73	1.12	0.54	0.38	0.90	0.23	
Th	-	-	-	-	-	-	-	-	-	
U	-	-	-	-	-	-	-	-	-	
V	-1.01	0.10	-1.03	-2.41	-1.43	0.10	0.86	-0.13	0.41	
Zn	0.00	0.25	0.46	1.03	0.93	-0.64	-1.20	-0.95	0.28	
Avg Deviat	0.13	0.10	0.16	0.22	0.25	0.24	0.26	0.20	0.33	

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

- As At MDL. Actually pretty good
- Cd Phase missing at high pH
- Co Actually pretty good
- Li Phase missing in pH 4-9 range
- Mg MgCO3 phase missing
- Mn Actually pretty good. Not easy to capture steep slope
- Mo Actually pretty good
- Ni Phase missing in pH 4 - 8 range. LDH-Ni?
- Pb Phase missing in pH 4 - 8 range. LDH-Ni?
- Se Proper phase missing
- Si Poor description.
- V At MDL. Actually pretty good
- Zn Reasonably good description over wide concentration range